

Bures geodesics and quantum metrology

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We study the geodesics on the manifold of mixed quantum states for the Bures metric. It is shown that these geodesics correspond to physical non-Markovian evolutions of the system coupled to an ancilla. Furthermore, we argue that geodesics lead to optimal precision in single-parameter estimation in quantum metrology. More precisely, if the unknown parameter x is a phase shift proportional to the time parametrizing the geodesic, the estimation error obtained by processing the data of measurements on the system is equal to the smallest error that can be achieved from joint detections on the system and ancilla, meaning that there is no information loss on this parameter in the ancilla. This error can saturate the Heisenberg bound. Reciprocally, assuming that the system-ancilla output and input states are related by a unitary e^{-ixH} with H a x -independent Hamiltonian, we show that if the error obtained from measurements on the system is equal to the minimal error obtained from joint measurements on the system and ancilla then the system evolution is given by a geodesic. In such a case, the measurement on the system bringing most information on x is x -independent and can be determined in terms of the intersections of the geodesic with the boundary of quantum states. These results show that geodesic evolutions are of interest for high-precision detections in systems coupled to an ancilla in the absence of measurements on the ancilla.

1 Introduction.

Geodesics play a prominent role in classical mechanics and general relativity as they describe the trajectories of free particles and light. In contrast, at first sight they are not relevant in quantum mechanics. In the quantum theory, the notion of trajectories in space or space-time has to be abandoned. Instead, quantum dynamics are described by time evolutions of quantum states. Such states are given by density matrices ρ forming a manifold of dimension $n^2 - 1$, where n is the dimension of the system Hilbert space $\mathcal{H}$ (which we assume here to be finite). Different distances can be defined on this manifold. A distance appearing natu-

rally in various contexts in quantum information theory is the Bures arccos distance d_B [1]. This distance is a good measure of the distinguishability of quantum states, being a simple function of the fidelity [2]. Furthermore, it has a clear information content, in particular it satisfies the data-processing inequality [1] and it is closely related to the quantum Fisher information quantifying the maximal amount of information on a parameter in a quantum state [3, 4]. Unlike the trace distance, d_B is a Riemannian distance, i.e., it has an associated metric g giving the square infinitesimal distance $ds^2 = (g_\rho)_{\alpha\beta} \partial_\alpha \rho \partial_\beta \rho$, where $\partial_\alpha \rho$ is the derivative of ρ with respect to the coordinate α and we make use of Einstein's summation convention. The manifold of quantum states $\mathcal{E}_{\mathcal{H}}$ equipped with the Bures metric is a Riemannian manifold, on which one can define geodesics.

In this work, we study these geodesics and analyze their usefulness in quantum metrology. Metrology is the science of devising schemes that extract as precise as possible estimates of the parameters associated to the system. In quantum metrology, the estimation of the unknown parameters (for instance, a phase shift in an interferometer) is obtained from the detection outcomes on quantum probes undergoing a parameter-dependent transformation process (for instance, the propagation in the two arms of the interferometer). It has been recognized that estimation errors scaling like the inverse of the number N of probes (Heisenberg limit) can be achieved using entangled probes, yielding an improvement by a factor of $1/\sqrt{N}$ with respect to the error for classical probes [5–12]. Quantum-enhanced precision have been observed experimentally in optical systems [13–15], trapped ions [16, 17], and Bose-Einstein condensates [18–20]. In these experiments, noise and losses lead to dephasing and entanglement losses, thus limiting the precision. In order to account for such limiting effects, several authors have studied parameter estimation in quantum systems coupled to their environment [22–32]. It has been argued that for dephasing and photon loss processes the $\sqrt{N}$ -improvement is lost, the best precision having the classical scaling for large N albeit with a better prefactor [21–27]. On the other hand, intermediate scalings $\sim N^{-\kappa}$ of the estimation error, with $1/2 \leq \kappa < 1$, have been obtained for phase-covariant and spin-boson models by optimizing not only the initial state but also the probe time [28, 29]. The results

of the aforementioned references are, however, model-dependent.

On a general ground, one expects that the environment coupling should increase the estimation error since information on the unknown parameter x can be lost in the environment and measurements on the latter are not possible. It is nevertheless known that, for any non-unitary transformation process on the probe, there exists an environment which does not deteriorate the precision of the estimation, i.e., a system-environment coupling such that no information on x is lost in the environment [25, 26]. Such a coupling depends in general on x . To determine it one must solve a non-trivial optimization problem.

In this paper we show that, in contrast to the aforementioned general expectation, it is possible to engineer parameter-independent coupling Hamiltonians of the probe with its environment such that there is no information losses on the estimated parameter x in the environment for any value of x , even though the coupling strongly entangles the probe and environment. Such a situation occurs when the transformation of the probe state is given by a Bures geodesic. As we shall see, the latter arises from a time evolution of the probe coupled to an ancilla with some specific coupling Hamiltonian, after tracing out the ancilla (i.e., the environment) degrees of freedom. The unknown parameter is a phase multiplying this Hamiltonian; it is proportional to the geodesic distance. For N probes coupled to independent ancillas, the precision on this phase saturates the Heisenberg bound, with an error $\sim N^{-1}$.

More precisely, we establish that (i) Bures geodesics are not purely mathematical objects but correspond to physical non-Markovian evolutions of the system coupled to an ancilla; we find explicitly the system-ancilla coupling Hamiltonian such that a state on the geodesic corresponds to the system state after an interaction with the ancilla during a lapse of time τ ; (ii) if the transformation process on a probe is given by a geodesic and the estimated parameter is a phase shift x proportional to the time τ parametrizing this geodesic, then the environment does not carry any information on x . This means that the estimation precision is equal to the best precision which can be achieved from joint measurements on the probe and ancilla, even if one can measure only the probe. Conversely, we show that system-ancilla Hamiltonians H with such a property always correspond to geodesics after tracing out the ancilla, if one moreover assumes that the input system-ancilla state achieves the best possible precision for H (this is in particular the case for N probes when the Heisenberg bound is saturated). We also show that (iii) there is an optimal measurement on the probes yielding the smallest error which is independent of the estimated parameter x and given in terms of the intersection states of the geodesic with the boundary $\partial\mathcal{E}_{\mathcal{H}}$ of the manifold of

quantum states.

As a consequence of (i), the geodesics are physical processes that can be simulated in quantum systems coupled to ancillas. We exhibit below examples of quantum circuits implementing some system-ancilla coupling Hamiltonians and corresponding geodesics. The geodesic evolutions being periodic in time, they are strongly non-Markovian, in the sense that memory effects and back action of the ancilla are important. Our results (ii) and (iii) show that geodesics are of practical interest in quantum metrology.

Our analysis relies on an application to the manifold of quantum states $\mathcal{E}_{\mathcal{H}}$ of the concept of Riemannian submersions in Riemannian geometry [33]. On the way, previous results in the literature [34, 35] on the explicit form of the Bures geodesics for arbitrary Hilbert space dimensions n are revisited. We show that these results are incomplete as they miss the geodesic curves joining two quantum states along paths which are not the shortest ones. We derive the explicit forms of all geodesics joining two invertible states ρ and σ at arbitrary dimensions n and study the intersections of these geodesics with the boundary $\partial\mathcal{E}_{\mathcal{H}}$. Moreover, we argue that the approach based on Riemannian geometry provides useful tools in quantum metrology.

The rest of the paper is organized as follows. A summary of our main results is presented in Sec. 2 after a brief introduction to quantum parameter estimation. The mathematical background on Riemannian geometry and submersions is given in Sec. 3. In Sec. 4, the explicit form of the Bures geodesics is derived and we study their intersections with the boundary $\partial\mathcal{E}_{\mathcal{H}}$. In Sec. 5, we show that the geodesics correspond to physical evolutions of the system coupled to an ancilla. The optimality of geodesics in quantum metrology is investigated in Sec. 6. Finally, our main conclusions and perspectives are drawn in Sec. 7. Two appendices contain some technical properties and proofs.

2 Main results

In this section we describe our main results and orient the reader to the subsequent sections, where these results are presented with more mathematical details.

2.1 Determination of the geodesics and their intersections with the boundary of quantum states

The explicit form of the Bures geodesics has been derived in Refs. [34, 35] for arbitrary Hilbert space dimensions $n < \infty$. The geodesic joining two invertible states ρ and σ determined in these references is given

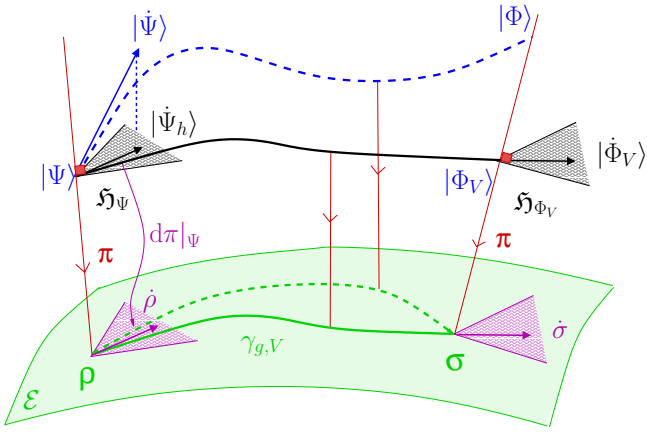


Figure 1: The manifold of quantum states $\mathcal{E} = \mathcal{E}_{\mathcal{H}}$ is the projection $\pi(\mathcal{S})$ of the manifold $\mathcal{S}$ of pure states on an enlarged Hilbert space $\mathcal{H} \otimes \mathcal{H}_A$, where π is the partial trace over $\mathcal{H}_A$. The horizontal subspaces at $|\Psi\rangle$ and $|\Phi_V\rangle$ are orthogonal to the orbits $\pi^{-1}(\rho)$ and $\pi^{-1}(\sigma)$ (red lines). A geodesic in $\mathcal{S}$ joining $|\Psi\rangle$ to $|\Phi_V\rangle$ (plain black curve) with a horizontal initial tangent vector $|\dot{\Psi}^h\rangle$ projects out to a geodesic $\gamma_{g,V}$ on $\mathcal{E}$ (green plain curve). In contrast, if the geodesic in $\mathcal{S}$ (blue dashed curve) has a non horizontal initial tangent vector, its projection (green dashed line) is not a geodesic on $\mathcal{E}$. The differential $d\pi$ maps the horizontal tangent vector $|\dot{\Psi}^h\rangle$ to a tangent vector $\dot{\rho}$ of $\gamma_{g,V}$ having the same length $\|\dot{\rho}\| = \|\dot{\Psi}^h\|$. A non horizontal vector $|\dot{\Psi}\rangle$ is mapped by $d\pi$ to a vector $\dot{\rho}$ with a smaller length, given by $\|\dot{\rho}\|^2 = \|\dot{\Psi}\|^2 - \|\dot{\Psi}^v\|^2$, where $|\dot{\Psi}^v\rangle$ is the vertical component of $|\dot{\Psi}\rangle$ (Pythagorean theorem).

by

$$\gamma_g(\tau) = \frac{1}{\sin^2 \theta} \left(\sin^2(\theta - \tau) \rho + \sin^2(\tau) \sigma + \sin(\theta - \tau) \sin(\tau) (\rho^{-1/2} |\sqrt{\sigma} \sqrt{\rho}| \rho^{1/2} + \text{h.c.}) \right) \quad (1)$$

with $0 \leq \tau \leq \theta = \arccos \sqrt{F(\rho, \sigma)}$, where $F(\rho, \sigma) = (\text{tr} |\sqrt{\sigma} \sqrt{\rho}|)^2$ is the fidelity between ρ and σ , $|O| = \sqrt{O^\dagger O}$ stands for the modulus of the operator O , and h.c. refers to the Hermitian conjugate. The geodesic (1) has a length θ equal to the arccos Bures distance $d_B(\rho, \sigma)$, it is thus the shortest geodesic arc joining ρ and σ . Recall that a curve is a geodesic if it has constant velocity and minimizes *locally* the length of curves between two points. In Riemannian manifolds, there exists in general geodesics joining two points which do not follow the shortest path from one point to the other. For instance, there are two geodesic arcs joining two non-diametrically opposite points on a sphere, namely the two arcs of the great circle passing through them; the smallest arc is the shortest geodesic, which minimizes the length globally, and the largest arc is another geodesic with a length strictly larger than the distance between its two extremities. On the other hand, if the two points on the sphere are diametrically opposite, there are infinitely many geodesics joining them, which have all

the same length.

In a similar way, we show in Sec. 4 that, depending on the two invertible mixed states ρ and σ , there is either a finite or an infinite number of Bures geodesics joining ρ and σ . The explicit form of these geodesics is given by a formula generalizing (1) in Theorem 1 below. For generic invertible states ρ and $\sigma \in \mathcal{E}_{\mathcal{H}}$, the number of geodesics is finite and equal to 2^n (recall that $n = \dim \mathcal{H}$). The geodesics can be classified according to the number of times they bounce on the boundary of quantum states $\partial \mathcal{E}_{\mathcal{H}}$ between ρ and σ . Recall that $\partial \mathcal{E}_{\mathcal{H}}$ is the set of non-invertible density matrices. The shortest geodesic (1) is the only geodesic starting at ρ and ending at σ without intersecting the boundary (but it does so if one extend it after σ , as shown in [34]).

Although these results are not the most original contribution of the paper, they form the starting point of the subsequent analysis. The method to determine the Bures geodesics is similar, albeit technically more involved, to textbook derivations of the Fubini-Study geodesics on the complex projective space $\mathbb{CP}^n$ (manifold of pure quantum states) [33]. It relies on the notion of Riemannian submersions. The main observation is that the manifold of (mixed) quantum states can be viewed as the projection of the manifold of pure states from an enlarged Hilbert space $\mathcal{H} \otimes \mathcal{H}_A$ (purifications), where $\mathcal{H}_A$ is an ancilla Hilbert space and the projection is the partial trace over the ancilla. The set of all purifications $|\Psi\rangle \in \mathcal{H} \otimes \mathcal{H}_A$ of ρ projecting out to the same density matrix ρ forms an orbit under the action of local unitaries on the ancilla. As noted by Uhlmann [2, 36], the Bures distance between ρ and σ is the norm distance between the corresponding orbits, that is, $d_{\text{Bures}}(\rho, \sigma) = \min \| |\Psi\rangle - |\Phi\rangle \|$ where the minimum is over all purifications $|\Psi\rangle$ and $|\Phi\rangle$ on the orbits of ρ and σ , respectively. For such a distance, the geodesics $\gamma_g(\tau)$ joining ρ and σ are obtained by projecting onto $\mathcal{E}_{\mathcal{H}}$ geodesics on the purification manifold having horizontal tangent vectors, as illustrated in Fig. 1. The latter geodesics are easy to determine since the metric on this manifold is the euclidean metric (given by the scalar product) restricted to a unit hypersphere (since purifications are normalized vectors). More details on Riemannian submersions are given in Sec. 3 below.

2.2 Geodesics correspond to physical evolutions

One of the purposes of this paper is to show that the Bures geodesics are not only mathematical objects but correspond to physical dynamical evolutions that could in principle be realized in the laboratory. Let $\gamma_g(\tau)$ be a geodesic on $\mathcal{E}_{\mathcal{H}}$ starting at $\rho = \gamma_g(0)$. Consider an ancilla system A with Hilbert space $\mathcal{H}_A$ of dimension $n_A \geq n$. Let $|\Psi\rangle$ be a purification of ρ on $\mathcal{H} \otimes \mathcal{H}_A$, i.e., $\rho = \text{tr}_A |\Psi\rangle\langle\Psi|$, where tr_A is the partial

trace over the ancilla. We show in Sec. 5 (see Theorem 2) that there exists a system-ancilla Hamiltonian H_g such that

$$\gamma_g(\tau) = \text{tr}_A e^{-i\tau H_g} |\Psi\rangle\langle\Psi| e^{i\tau H_g}. \quad (2)$$

In other words, $\gamma_g(\tau)$ is the system state at the (dimensionless) time τ , given that the system is coupled to the ancilla at time 0 and interacts with it up to time τ with the Hamiltonian H_g . This Hamiltonian reads

$$H_g = -i(|\Psi\rangle\langle\dot{\Psi}| - |\dot{\Psi}\rangle\langle\Psi|), \quad (3)$$

where $|\dot{\Psi}\rangle$ is a normalized vector satisfying the horizontality condition

$$|\dot{\Psi}\rangle = L_S \otimes \mathbb{1}_A |\Psi\rangle \quad (4)$$

for some self-adjoint operator L_S acting on the system such that $\langle L_S \otimes \mathbb{1}_A \rangle_\Psi = 0$. Condition (4) can be interpreted geometrically as follows: $|\dot{\Psi}\rangle$ is a vector in the tangent space at $|\Psi\rangle$ which is orthogonal to the orbit $\{\mathbb{1} \otimes U_A |\Psi\rangle; U_A \text{ unitary on } \mathcal{H}_A\}$ of ρ under the unitary group on the ancilla. Note that $\langle \Psi | \dot{\Psi} \rangle = 0$. As will be shown in Sec. 6, the operator $2L_S$ is equal to the symmetric logarithmic derivative of $\gamma_g(\tau)$ at $\tau = 0$.

Since ρ can be chosen arbitrarily on γ_g and all geodesics extended over the time interval $[0, \pi]$ intersect the boundary of quantum states $\partial\mathcal{E}_\mathcal{H}$ (see Appendix B), one can without loss of generality assume that $\rho \in \partial\mathcal{E}_\mathcal{H}$. If γ_g has an intersection with $\partial\mathcal{E}_\mathcal{H}$ given by a pure state $\rho_\psi = |\psi\rangle\langle\psi|$, one can choose $\rho = \rho_\psi$. Then the purifications of ρ are product states $|\Psi\rangle = |\psi\rangle|\alpha\rangle$ and, as a consequence of (2), there is a smooth family of Completely Positive Trace Preserving (CPTP) maps $\mathcal{M}_{g,\tau}$ (quantum channels) such that

$$\gamma_g(\tau) = \mathcal{M}_{g,\tau}(\rho), \quad (5)$$

i.e., the geodesic evolution is obtained by applying $\mathcal{M}_{g,\tau}$ to ρ . The quantum evolution $\{\mathcal{M}_{g,\tau}\}_{\tau \geq 0}$ is strongly non-Markovian. Actually, we show in Sec. 5 that this evolution is periodic in time,

$$\mathcal{M}_{g,\tau+2\pi} = \mathcal{M}_{g,\tau}. \quad (6)$$

For a system formed by d qubits coupled to d ancilla qubits, the geodesics can be implemented by the quantum circuit of Fig. 2(a), where U_{SA} is a unitary operator on $\mathcal{H} \otimes \mathcal{H}_A$ such that

$$|\Psi\rangle = U_{SA}|0\rangle|0\rangle_A, \quad |\dot{\Psi}\rangle = U_{SA}|1\rangle|0\rangle_A. \quad (7)$$

Here, $\{|k\rangle\}_{k=0}^{n-1}$ and $\{|k\rangle_A\}_{k=0}^{n-1}$ denotes the computational bases of $\mathcal{H} \simeq \mathbb{C}^n$ and $\mathcal{H}_A \simeq \mathbb{C}^n$ (with $n = 2^d$). Indeed, denoting by $\sigma_y^{(1)}$ the y -Pauli matrix acting on the first qubit and by $\mathbb{1}^{(2\dots d)}$ the identity operator on the other qubits of the system, the Hamiltonian

$$\tilde{H}_g = U_{SA} \sigma_y^{(1)} \otimes \mathbb{1}^{(2\dots d)} \otimes \mathbb{1}_A U_{SA}^\dagger \quad (8)$$

leaves the subspace $\text{span}\{|\Psi\rangle, |\dot{\Psi}\rangle\}$ invariant and coincides with the geodesic Hamiltonian (3) on this subspace. Thus

$$e^{-i\tau H_g} |\Psi\rangle = U_{SA} e^{-i\tau \sigma_y^{(1)}} \otimes \mathbb{1}^{(2\dots d)} \otimes \mathbb{1}_A |0\rangle|0\rangle_A. \quad (9)$$

By (2), the state of the system at the output of the circuit is $\gamma_g(\tau)$. The two circuits of Fig. 2(b) and (c) give examples of entangling unitaries U_{SA} implementing a geodesic $\gamma_g(\tau)$ through an arbitrary invertible state $\rho = \gamma_g(0)$. Introducing the spectral decomposition $\rho = \sum_k p_k |w_k\rangle\langle w_k|$, one checks that (7) holds for both circuits, with $|\Psi\rangle = \sum_k \sqrt{p_k} |w_k\rangle |k\rangle_A$ a purification of ρ and $|\dot{\Psi}\rangle$ a horizontal tangent vector of the form (4) for some self-adjoint operator L_S . Note that the system-ancilla entangling operation in these circuits is obtained by means of d C-NOT gates. The geodesic implemented by the unitary U_{SA} of Fig. 2(b) is a geodesic joining two commuting states (see Sec. 4).

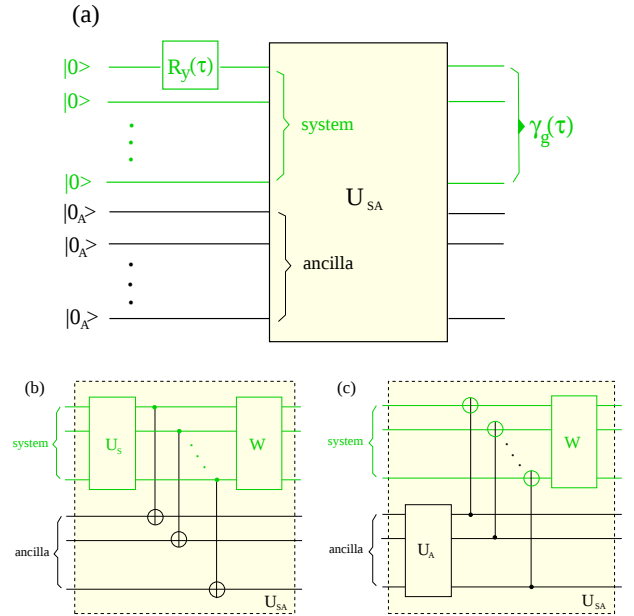


Figure 2: Quantum circuit implementing the geodesic evolution. (a): General circuit for a d -qubit system; $R_y(\tau) = e^{-i\tau \sigma_y}$ is a rotation around the y -axis and U_{SA} is a system-ancilla entangling unitary satisfying (7). (b), (c): examples of quantum circuits for U_{SA} ; the unitaries W , U_S , and U_A are such that $U_i|0\rangle_i = \sum_k \sqrt{p_k} |k\rangle_i$, $i = S, A$, $U_S|1\rangle_S = \sum_k \alpha_k |k\rangle$, and $W|k\rangle_S = |w_k\rangle_S$, $k = 0, \dots, 2^d - 1$, where $\sqrt{p_k}$ and $\{|w_k\rangle_S\}$ are the coefficients and orthonormal basis in the Schmidt decomposition of $|\Psi\rangle$ and $\alpha_k \in \mathbb{R} \setminus \{0\}$, $\sum_k \alpha_k \sqrt{p_k} = 0$.

2.3 Optimality of geodesics for parameter estimation in open quantum systems

Before explaining our results, let us introduce some basic background on quantum metrology for readers not familiar with this field. More information can be found e.g. in the review articles [3, 8, 12, 37].

Parameter estimation in closed and open quantum systems.

The goal of parameter estimation is to estimate an unknown real parameter x pertaining to an interval $X \subset \mathbb{R}$ by performing measurements on a quantum system (probe). Before each measurement, the system undergoes a x -dependent process transforming the input state ρ_{in} into an output state ρ_x . The estimator $x_{\text{est}} \in X$ is a function of the measurement outcomes. The precision of the estimation is characterized by the variance $(\Delta x)^2 = \langle (x_{\text{est}} - x)^2 \rangle_x$, where $\langle \cdot \rangle_x$ refers to the average over the outcomes conditioned to the parameter value x . Hereafter, we assume that the estimator is locally unbiased, i.e., $\langle x_{\text{est}} \rangle_x = x$ and $\partial_x \langle x_{\text{est}} \rangle_x = 1$. Furthermore, we assume that the map $x \in X \mapsto \rho_x$ is injective and that ρ_x has a rank independent of x . If one performs N_{meas} independent identical measurements on identical probes prepared in state ρ_x , then the estimation error satisfies the quantum Crámer-Rao bound [39, 40]

$$\Delta x \geq (\Delta x)_{\text{QCRB}} = \frac{1}{\sqrt{N_{\text{meas}} \mathcal{F}_Q(x, \{\rho_x\}_{x \in X})}}, \quad (10)$$

where $\mathcal{F}_Q(x, \{\rho_x\}_{x \in X})$ is the quantum Fisher information (QFI). The QFI is obtained by maximizing over all measurements the classical Fisher information (CFI)

$$\mathcal{F}_{\text{clas}}(x, \{p_{j|x}\}_{x \in X}) = \sum_{j, p_{j|x} > 0} \frac{(\partial_x p_{j|x})^2}{p_{j|x}}, \quad (11)$$

where $p_{j|x}$ is the probability of the measurement outcome j given that the system is in state ρ_x . Note that the QFI and CFI depend on general on the parameter value x . For clarity we write this dependence on x explicitly. The bound (10) is saturated asymptotically (in the limit $N_{\text{meas}} \gg 1$) by choosing: (i) the maximum likelihood estimator x_{est} (ii) the optimal measurement maximizing the CFI, for which $\mathcal{F}_{\text{clas}} = \mathcal{F}_Q$. This means that the right-hand side of (10) gives the smallest error that can be achieved in the estimation. Note that this result is not true if the map $x \in X \mapsto \rho_x$ is not injective, because different values of x corresponding to the same ρ_x can not be distinguished. To circumvent this problem, one can partition the interval X into smaller intervals X_k such that $x \in X_k \mapsto \rho_x$ is injective for each k , provided one has some prior knowledge about the X_k to which x belongs [12]. The saturation of the bound (10) and the bound itself may also not be true when the rank of ρ_x has a jump at the parameter value x , see e.g. [42].

Using classical resources, the smallest estimation error $(\Delta x)_{\text{QCRB}}$ scales with the number of probes N like $1/\sqrt{N}$ (shot noise limit). Multipartite entanglement among the quantum probes can enhance the precision by a factor $1/\sqrt{N}$, leading to errors $(\Delta x)_{\text{QCRB}}$ scaling like $1/N$ (Heisenberg limit) [5–11].

For a closed system in a pure state undergoing the x -dependent unitary transformation $|\Psi_x\rangle =$

$e^{-ixH}|\Psi_{\text{in}}\rangle$, where H is a given observable, the QFI is given by [4, 40]

$$\begin{aligned} \mathcal{F}_Q(\{|\Psi_x\rangle_{x \in X}\}) &= 4(\|\dot{\Psi}_x\|^2 - |\langle \Psi_x | \dot{\Psi}_x \rangle|^2) \\ &= 4\langle (\Delta H)^2 \rangle_{\Psi_{\text{in}}}, \end{aligned} \quad (12)$$

where $|\dot{\Psi}_x\rangle$ is the derivative of $|\Psi_x\rangle$ with respect to x and $\langle (\Delta H)^2 \rangle_{\Psi} = \langle \Psi | H^2 | \Psi \rangle - \langle \Psi | H | \Psi \rangle^2$ is the square quantum fluctuation of H in state $|\Psi\rangle$. The input states maximizing this fluctuation are the superpositions

$$|\Psi_{\text{in}}\rangle = \frac{1}{\sqrt{2}}(|\epsilon_{\text{max}}\rangle + e^{i\varphi}|\epsilon_{\text{min}}\rangle), \quad (13)$$

where φ is a real phase and $|\epsilon_{\text{max}}\rangle$ (respectively $|\epsilon_{\text{min}}\rangle$) is an eigenstate of H with maximal (minimal) eigenvalue ϵ_{max} (ϵ_{min}). (We assume here that these eigenvalues are non-degenerated.) The corresponding maximal QFI is $\mathcal{F}_Q(\{|\Psi_x\rangle_{x \in X}\}) = 4\epsilon^2$ with $\epsilon = (\epsilon_{\text{max}} - \epsilon_{\text{min}})/2$. According to (10) and (12), the states (13) are the optimal input states minimizing the estimation error $(\Delta x)_{\text{QCRB}}$. Indeed, by convexity of the QFI, using mixed input states ρ_{in} can not lead to smaller errors. Note that the QFI (12) is independent of x , as clear from the last expression. For this reason, we omit x in the argument of $\mathcal{F}_Q$. In contrast, for non-unitary evolutions the QFI depends in general upon the value x of the estimated parameter.

For N probes undergoing a unitary “parallel” transformation with the observable $H_N = \sum_{i=1}^N H_i$, where H_i stands for the action of H on the i th probe, the error has the Heisenberg scaling $(\Delta x)_{\text{QCRB}} \propto 1/N$ (more precisely, $(\Delta x)_{\text{QCRB}} = (2N\epsilon\sqrt{N_{\text{meas}}})^{-1}$). The optimal input states, given by replacing $|\epsilon_{\text{max}}\rangle$ and $|\epsilon_{\text{min}}\rangle$ in (13) by the eigenvectors of H_N with maximal and minimal eigenvalues $N\epsilon_{\text{max}}$ and $N\epsilon_{\text{min}}$, show genuine multipartite entanglement.

In experimental setups, the coupling of the probes with their environment can not be neglected. A general description of the state transformation process is given by a family $\{\mathcal{M}_x\}_{x \in X}$ of x -dependent quantum channels, which accounts for the joint effects of the free evolutions of the probe $\mathbf{P}$ and environment $\mathbf{E}$ and the coupling between them. The probe output state is related to the input state ρ_{in} by

$$\rho_x = \mathcal{M}_x(\rho_{\text{in}}). \quad (14)$$

In a realistic scenario, measurements can be performed on the probe only, i.e., one can not extract information from the environment. The error $(\Delta x)_{\text{QCRB}}$ obtained by measuring the probe can clearly not be smaller than the error $(\Delta x)_{\text{QCRB,PE}}$ obtained from joint measurements on the probe and environment. A natural question is whether there exists a family of quantum channels $\{\mathcal{M}_x\}_{x \in X}$ and input states $|\Psi_{\text{in}}\rangle$ such that $(\Delta x)_{\text{QCRB}} = (\Delta x)_{\text{QCRB,PE}}$ for any value of x . This means that the environment does not carry any information about the parameter x .

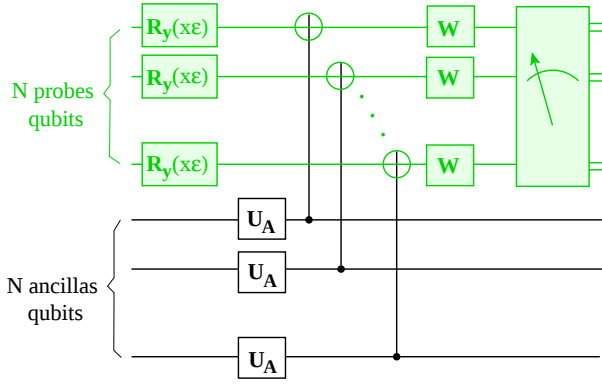


Figure 3: Quantum circuit implementing a geodesic transformation for the estimation of a phase shift x , with an error reaching the Heisenberg scaling. The single qubit unitaries R_y , U_A and W are as in Fig. 2 with $d = 1$. In spite of the presence of the C-NOT gates entangling the probe qubits with the ancilla qubits, the maximal information on x can be recovered from measurements on the probe qubits only, with a minimal error $(\Delta x)_{\text{QCRB}} = (2N\epsilon\sqrt{N_{\text{meas}}})^{-1}$.

Optimality of geodesics in parameter estimation.

We will show in Sec. 6 below that it is possible to find such a family of quantum channels and input state, which are moreover such that the error $(\Delta x)_{\text{QCRB}}$ is equal to the smallest possible error

$$(\Delta x)_{\text{QCRB}} = (\Delta x)_{\text{QCRB,PE}} = (2N\epsilon\sqrt{N_{\text{meas}}})^{-1}, \quad (15)$$

where $\epsilon = (\epsilon_{\text{max}} - \epsilon_{\text{min}})/2$ is as before the maximal quantum fluctuation of the observable H . Such a family is given by the CPTP maps associated to the Bures geodesics described in the previous subsection. The corresponding state transformation is

$$\rho_x = \gamma_g(x\epsilon), \quad (16)$$

where $\gamma_g(\tau)$ is a geodesic starting at

$$\gamma_g(0) = \rho_{\text{in}} = \text{tr}_A |\Psi_{\text{in}}\rangle\langle\Psi_{\text{in}}|. \quad (17)$$

Note that the estimated parameter x appears in (16) as a phase shift proportional to the dimensionless time τ , and that γ_g is an arbitrary *fixed* geodesic passing through ρ_{in} .

In other words, for the state transformation and phase shift x given in (16), one has: (i) the precision on the estimation of x obtained from measurements on the probe only is the same as that obtained by performing joint measurements on the probe and environment; (ii) the error $(\Delta x)_{\text{QCRB}} = (\Delta x)_{\text{QCRB,PE}}$ is the smallest achievable among all probe-environment initial states. Furthermore, the error scales like N^{-1} with the number of probes, i.e., it reaches the Heisenberg bound. An example of quantum circuit implementing the corresponding state transformation is shown in Fig. 3.

To justify properties (i)-(ii), let us look at the transformation (14) as resulting from the coupling of the

probe with an ancilla A, the probe and ancilla being initially in a pure state and undergoing a unitary transformation. Note that this is always possible according to Stinespring's theorem [38]. Let us assume that the unitary evolution of the probe and ancilla is generated by some x -independent Hamiltonian H . Thus

$$\rho_x = \text{tr}_A |\Psi_x\rangle\langle\Psi_x|, \quad |\Psi_x\rangle = e^{-ixH} |\Psi_{\text{in}}\rangle. \quad (18)$$

Using the physical irrelevance of phase factors in the quantum states $|\Psi_x\rangle$, we may assume that $\langle H \rangle_{\text{in}} = \langle \Psi_{\text{in}} | H | \Psi_{\text{in}} \rangle = 0$ (in fact, this amounts to multiply $|\Psi_x\rangle$ by the phase factor $e^{ix\langle H \rangle_{\text{in}}}$, i.e., to replace H by $\Delta H = H - \langle H \rangle_{\text{in}}$ in (18)). Let us decompose the tangent vector $|\dot{\Psi}_x\rangle = \partial_x |\Psi_x\rangle$ into the sum of its horizontal part $|\dot{\Psi}_x^h\rangle$ and its vertical part $|\dot{\Psi}_x^v\rangle$, with $\langle \dot{\Psi}_x^h | \dot{\Psi}_x^v \rangle = 0$, where horizontality means orthogonality to the orbit of ρ_x , see Fig. 1. According to the theory of Riemannian submersions, the square norm of the horizontal part coincides with the square norm $(g_B)_{\rho_x}(\dot{\rho}_x, \dot{\rho}_x)$ of $\dot{\rho}_x = \partial_x \rho_x$, the latter norm being given by the Bures metric g_B at ρ_x (see Sec. 3). It is known that this square norm is equal to the QFI up to a factor of one fourth [4, 40]. Thus, thanks to the Pythagorean theorem $\|\dot{\Psi}_x\|^2 = \|\dot{\Psi}_x^h\|^2 + \|\dot{\Psi}_x^v\|^2$, one obtains the following formula for the QFI of the probe [25]

$$\mathcal{F}_Q(x, \{\rho_x\}_{x \in X}) = \mathcal{F}_Q(\{|\Psi_x\rangle\}_{x \in X}) - 4\|\dot{\Psi}_x^v\|^2, \quad (19)$$

where the QFI of the total system (probe and ancilla) is given by $\mathcal{F}(\{|\Psi_x\rangle\}_{x \in X}) = 4\|\dot{\Psi}_x\|^2$ thanks to (12) and our assumption $\langle H \rangle_{\text{in}} = 0$, and $\|\dot{\Psi}_x^v\|^2$ quantifies the amount of information on x in the ancilla. It follows that the equality $\mathcal{F}_Q(x, \{\rho_x\}_{x \in X}) = \mathcal{F}_Q(\{|\Psi_x\rangle\}_{x \in X})$ holds whenever $|\dot{\Psi}_x^v\rangle = 0$, i.e., for horizontal tangent vectors $|\dot{\Psi}_x\rangle$.

Let $|\Psi_g(\tau)\rangle$ be a pure-state geodesic for the norm distance on $\mathcal{K} = \mathcal{H} \otimes \mathcal{H}_A$. A general result on Riemannian submersions tells us that if the tangent vector $|\dot{\Psi}_g(\tau)\rangle$ is horizontal at $\tau = 0$ then it remains horizontal at all times τ and $|\Psi_g(\tau)\rangle$ projects out to a geodesic $\gamma_g(\tau)$ on $\mathcal{E}_{\mathcal{H}}$, where the projection corresponds here to the partial trace over the ancilla (see Sec. 3.3 for more details). Reciprocally, any geodesic on $\mathcal{E}_{\mathcal{H}}$ can be lifted locally to a pure-state geodesic $|\Psi_g(\tau)\rangle$ with horizontal tangent vectors. Therefore, for the state transformation (16) one has $|\dot{\Psi}_x^v\rangle = 0$ for all parameter values x . Thanks to (10) and (19), $(\Delta x)_{\text{QCRB}}$ is then equal to the best error obtained from measurements on the probe and ancilla. This justifies property (i) above. Furthermore, it is easy to show that $|\Psi_{\text{in}}\rangle$ is the superposition (13) for the Hamiltonian $H = \epsilon H_g$, H_g being given by (3) with $|\Psi\rangle = |\Psi_{\text{in}}\rangle$ and $|\dot{\Psi}\rangle = |\dot{\Psi}_{\text{in}}\rangle/\|\dot{\Psi}_{\text{in}}\|$ (note that our hypothesis $\langle H \rangle_{\text{in}} = 0$ is fulfilled for this Hamiltonian). This justifies (ii).

Conversely, we show in Sec. 6 that if the state transformation of the probe and ancilla is given by a unitary $U_x = e^{-ixH}$, where x is the unknown parameter

and H a parameter-independent Hamiltonian, and if properties (i) and (ii) hold, then the state transformation of the probe is necessarily a geodesic evolution. More precisely, Theorem 3 characterizes all Hamiltonians H and input states $|\Psi_{\text{in}}\rangle$ of the probe and ancilla satisfying the two following conditions, which are equivalent to (i) and (ii): (I) $|\Psi_x\rangle$ is horizontal for all $x \in X$ (i.e., it satisfies (4)); (II) the QFI of the probe and ancilla is maximal (i.e., $\mathcal{F}(\{|\Psi_x\rangle\}_{x \in X}) = 4N^2\epsilon^2$). We prove that these conditions hold if and only if $|\Psi_x\rangle = |\Psi_g(x\epsilon)\rangle = e^{-ix\epsilon H_g}|\Psi_{\text{in}}\rangle$ is a pure-state geodesic of the probe and ancilla with a horizontal initial tangent vector $|\dot{\Psi}_{\text{in}}\rangle$, i.e., if and only if the state transformation has the form (16) for some geodesic γ_g and initial state (17). By (19), this implies that geodesic evolutions are optimal for quantum parameter estimation in the following sense: among all coupling Hamiltonians H of the probe and ancilla having a fixed energy gap 2ϵ and all initial states $|\Psi_{\text{in}}\rangle$ satisfying (II), the highest QFI of the probe for arbitrary parameter values x is obtained when H generates a geodesic evolution of the probe. As we show in Sec. 6, this occurs when the restriction of H to the two-dimensional subspace spanned by its eigenvectors associated to the maximal and minimal eigenvalues coincides with the geodesic Hamiltonian (3) multiplied by ϵ , with $|\Psi\rangle = |\Psi_{\text{in}}\rangle$ and $|\dot{\Psi}\rangle = |\dot{\Psi}_{\text{in}}\rangle/\|\dot{\Psi}_{\text{in}}\|$. Theorem 4 shows that these eigenvectors must be related by $|\epsilon_{\text{min}}\rangle = U \otimes \mathbb{1}|\epsilon_{\text{max}}\rangle$ for some local unitary U acting on the probe.

Another nice property of the state transformation (16) is related to the optimal measurement. Recall that a measurement is given by a POVM $\{M_j\}$, that is, a set of non-negative operators $M_j \geq 0$ on $\mathcal{H}$ such that $\sum_j M_j = \mathbb{1}$. The outcome probabilities when the system is in state ρ_x are given by $p_{j|x} = \text{tr } M_j \rho_x$. An optimal measurement is a POVM $\{M_j^{\text{opt}}\}$ for which the CFI (11) coincides with the QFI. Such a measurement leads to the smallest error $\Delta x = (\Delta x)_{\text{QCRB}}$ in (10). In general, $\{M_j^{\text{opt}}\}$ depends on the parameter x [3]. Since x is unknown *a priori*, it is then in practice impossible to implement directly an optimal measurement strategy. A notable exception is a closed system undergoing a unitary transformation with an input state given by the superposition (13) minimizing the error. Then the optimal measurement is independent of x . Theorem 5 in Sec. 6 shows that the geodesic transformation (16) enjoys the same property. More precisely, one has: (iii) there is an optimal POVM $\{M_j^{\text{opt}}\}$ maximizing the CFI which is independent of x and is given by the von Neumann measurement with projectors onto $\ker \rho_j$, where ρ_j are the states at which the geodesic γ_g intersects the boundary $\partial\mathcal{E}_{\mathcal{H}}$ of quantum states. This property gives a practical way to determine an optimal measurement in numerical simulations or experiments: first determine the smallest eigenvalue $p_n(x) = \min_{\|\psi\|=1} \langle \psi | \rho_x | \psi \rangle$ of ρ_x for different values of x until finding a parameter value x_j such

that $p_n(x_j) \simeq 0$ (if x is random and can not be tuned, just repeat the transformation many times); then determine all eigenvalues very close to zero of $\rho_j = \rho_{x_j}$ and the associated eigenvectors (this can be done by minimization of $\langle \psi | \rho_j | \psi \rangle$ in orthogonal subspaces, or by using quantum state tomography); repeat this procedure for different values of x_j until obtaining an orthonormal basis of $\mathcal{H}$ formed by eigenvectors of the states ρ_j with vanishing eigenvalues. Note that Theorem 6 in Appendix B shows that these eigenvectors indeed form an orthonormal basis. Then such a basis is an optimal measurement basis for the estimation of x .

Let us comment that the geometric approach described in the following sections is not restricted to geodesic evolutions and provides a new method for studying parameter estimation in open quantum systems. Actually, the above arguments show that, for a fixed QFI of the probe and environment (i.e., a fixed value of the square fluctuation $\langle (\Delta H)^2 \rangle_{\Psi_{\text{in}}}$), one can enhance the QFI of the probe and thus the precision of the estimation by reducing the vertical component of the tangent vector $|\dot{\Psi}_x\rangle = -i\Delta H|\Psi_x\rangle$, see (19). Given a Hamiltonian H of the probe and environment, the direction of $|\dot{\Psi}_x\rangle$ could be changed using control techniques on the probe or its environment, to make $|\dot{\Psi}_x\rangle$ more horizontal while keeping its norm fixed. This may be useful for designing new engineering reservoir techniques in order to increase precision in quantum metrology in the presence of losses and dephasing.

3 Mathematical preliminaries

In this section we describe the geometrical properties of the manifold of mixed states of a quantum system equipped with the Bures distance and introduce the notion of Riemannian submersions.

3.1 Riemannian geometry for quantum states and Bures distance.

Let us first recall some basic notions of Riemannian geometry. A metric on a smooth manifold $\mathcal{E}$ is a smooth map g associating to each point $\rho \in \mathcal{E}$ a scalar product g_ρ on the tangent space $T_\rho\mathcal{E}$ at ρ . A curve γ on $\mathcal{E}$ joining two points ρ and σ is parametrized by a piecewise C^1 map $\gamma : t \in [t_0, t_1] \mapsto \gamma(t) \in \mathcal{E}$ such that $\gamma(t_0) = \rho$ and $\gamma(t_1) = \sigma$. Its length $\ell(\gamma)$ is

$$\ell(\gamma) = \int_\gamma ds = \int_{t_0}^{t_1} dt \sqrt{g_{\gamma(t)}(\dot{\gamma}(t), \dot{\gamma}(t))}, \quad (20)$$

where $\dot{\gamma}(t)$ stands for the time derivative $d\gamma/dt$. A Riemannian distance d on $\mathcal{E}$ can be associated to any metric g , defined as the infimum $d(\rho, \sigma) = \inf_\gamma \ell(\gamma)$ of the lengths of all curves γ joining ρ and σ . Such a distance is called the geodesic distance on $(\mathcal{E}, g)$. Curves γ_g with constant velocity minimizing the length *locally*

are called geodesics. More precisely, $\gamma_g : [t_0, t_1] \rightarrow \mathcal{E}$ is a geodesic if (i) $g_{\gamma_g(t)}(\dot{\gamma}_g(t), \dot{\gamma}_g(t)) = \text{const.}$ and (ii) $\forall t \in (t_0, t_1), \exists \delta > 0$ such that $\ell(\gamma_g|_{[t, t+\delta]}) = d(\gamma_g(t), \gamma_g(t+\delta))$. In particular, if there is a geodesic γ_g with length $\ell(\gamma_g) = d(\rho, \sigma)$ minimizing the length globally, one says that γ_g is the shortest geodesic joining ρ and σ .

Conversely, one can associate to a distance d on $\mathcal{E}$ a metric g if d satisfies the following condition (we ignore here regularity assumptions): for any $\rho \in \mathcal{E}$ and $\dot{\rho} \in T_\rho \mathcal{E}$, the square distance between ρ and $\rho + t\dot{\rho}$ behaves as $t \rightarrow 0$ as

$$ds^2 = d(\rho, \rho + t\dot{\rho})^2 = g_\rho(\dot{\rho}, \dot{\rho})t^2 + \mathcal{O}(t^3). \quad (21)$$

In quantum mechanics, states are represented by non-negative operators ρ with unit trace from the Hilbert space $\mathcal{H}$ of the system into itself. We assume hereafter that $\mathcal{H}$ has finite dimension $n = \dim(\mathcal{H}) < \infty$ and denote by $\mathcal{E}_\mathcal{H}$ the set of all quantum states of a given system. The arccos Bures distance between two states ρ and σ is defined by [1]

$$d_B(\rho, \sigma) = \arccos \sqrt{F(\rho, \sigma)}, \quad (22)$$

where

$$F(\rho, \sigma) = \left(\text{tr}(\sqrt{\sigma} \sqrt{\rho}) \right)^2 = \left(\text{tr}(\sqrt{\rho} \sigma \sqrt{\rho})^{\frac{1}{2}} \right)^2 \quad (23)$$

is the fidelity. The set of all invertible states,

$$\mathcal{E}_\mathcal{H}^{\text{inv}} = \{ \rho : \mathcal{H} \rightarrow \mathcal{H}, ; \rho > 0, \text{tr} \rho = 1 \}, \quad (24)$$

equipped with the distance d_B forms a smooth open Riemannian manifold. Its boundary $\partial \mathcal{E}_\mathcal{H}$ consists of density matrices ρ having at least one vanishing eigenvalue; for instance, pure states $\rho_\psi = |\psi\rangle\langle\psi|$ are on the boundary.

The tangent space at $\rho \in \mathcal{E}_\mathcal{H}^{\text{inv}}$ can be identified with the (real) vector space of self-adjoint traceless operators on $\mathcal{H}$,

$$T_\rho \mathcal{E}_\mathcal{H} = \{ \dot{\rho} : \mathcal{H} \rightarrow \mathcal{H}, \dot{\rho}^\dagger = \dot{\rho}, \text{tr} \dot{\rho} = 0 \}. \quad (25)$$

The metric g_B associated to the distance d_B is given explicitly by [4, 44]

$$(g_B)_\rho(\dot{\rho}, \dot{\sigma}) = \frac{1}{2} \text{Re} \sum_{k,l=1}^n \frac{\langle k|\dot{\rho}|l\rangle \langle k|\dot{\sigma}|l\rangle}{p_k + p_l}, \quad \dot{\rho}, \dot{\sigma} \in T_\rho \mathcal{E}_\mathcal{H}, \quad (26)$$

where $\{|k\rangle\}_{k=1}^n$ is an orthonormal basis of eigenvectors of ρ with eigenvalues p_k .

3.2 Purifications and smooth submersions

Mixed quantum states of a given system can be described by introducing an auxiliary system A, called the ancilla, and viewing the system state ρ as the reduced state of the system + ancilla. The dimension of the ancilla Hilbert space $\mathcal{H}_A$ is assumed to fulfill

$n_A \geq n$. We denote by $\mathcal{K} = \mathcal{H} \otimes \mathcal{H}_A$ the Hilbert space of the composite system. A purification of ρ on $\mathcal{K}$ is a pure state $|\Psi\rangle\langle\Psi|$ such that $|\Psi\rangle \in \mathcal{K}$ and $\rho = \pi(|\Psi\rangle)$, with

$$\pi(|\Psi\rangle) = \text{tr}_A |\Psi\rangle\langle\Psi|, \quad (27)$$

where tr_A stands for the partial trace over the ancilla space $\mathcal{H}_A$. For our purpose, it is convenient to consider purifications as normalized vectors in $|\Psi\rangle \in \mathcal{K}$, instead of pure states (recall that a pure state is a normalized vector modulo a phase factor and can be represented as a rank-one projector $|\Psi\rangle\langle\Psi|$ in the projective space $P\mathcal{K}$). The condition $\rho > 0$ is satisfied if and only if $|\Psi\rangle$ has Schmidt decomposition

$$|\Psi\rangle = \sum_{k=1}^n \sqrt{p_k} |k\rangle |\alpha_k\rangle \quad (28)$$

with n positive Schmidt coefficients $\sqrt{p_k} > 0$, $k = 1, \dots, n$. Here, $\{|k\rangle\}_{k=1}^n$ is an orthonormal eigenbasis of ρ and $\{|\alpha_k\rangle\}_{k=1}^{n_A}$ is an arbitrary orthonormal basis of $\mathcal{H}_A$. The set of purifications of invertible states is thus the subset of the unit sphere in $\mathcal{K}$ given by

$$\mathcal{S}_\mathcal{K}^{\text{inv}} = \{ |\Psi\rangle \in \mathcal{K} ; \|\Psi\| = 1, |\Psi\rangle \text{ has } n \text{ positive Schmidt coefficients} \}. \quad (29)$$

The tangent space of $\mathcal{S}_\mathcal{K}^{\text{inv}}$ at $|\Psi\rangle \in \mathcal{S}_\mathcal{K}^{\text{inv}}$ is

$$T_{|\Psi\rangle} \mathcal{S}_\mathcal{K} = \{ |\dot{\Psi}\rangle \in \mathcal{K} ; \text{Re} \langle \Psi | \dot{\Psi} \rangle = 0 \}. \quad (30)$$

A natural metric on $\mathcal{S}_\mathcal{K}^{\text{inv}}$ is $g_S(|\dot{\Psi}\rangle, |\dot{\Phi}\rangle) = \text{Re} \langle \dot{\Psi} | \dot{\Phi} \rangle$. Note that the scalar product is independent of $|\Psi\rangle$. This metric is that induced by the euclidean metric on $\mathcal{K}$. The Riemannian manifold $(\mathcal{S}_\mathcal{K}^{\text{inv}}, g_S)$ is isometric under the action $|\Psi\rangle \mapsto \mathbb{1} \otimes U_A |\Psi\rangle$ of the unitary group $U(n_A)$ acting on the ancilla, that is,

$$g_S(\mathbb{1} \otimes U_A |\dot{\Psi}\rangle, \mathbb{1} \otimes U_A |\dot{\Phi}\rangle) = g_S(|\dot{\Psi}\rangle, |\dot{\Phi}\rangle) \quad (31)$$

for any unitary U_A on $\mathcal{H}_A$.

We now argue that $\mathcal{E}_\mathcal{H}^{\text{inv}}$ can be viewed as the quotient of $\mathcal{S}_\mathcal{K}^{\text{inv}}$ by the unitary group $U(n_A)$. The map (27) defines a projection from $\mathcal{S}_\mathcal{K}^{\text{inv}}$ onto $\mathcal{E}_\mathcal{H}^{\text{inv}}$. The set $\pi^{-1}(\rho)$ of all purifications of ρ coincides with the orbit of ρ under the group action,

$$\pi^{-1}(\rho) = \{ |\Psi\rangle = \mathbb{1} \otimes U_A |\Psi_0\rangle ; U_A \text{ unitary on } \mathcal{H}_A \}, \quad (32)$$

where $|\Psi_0\rangle \in \mathcal{S}_\mathcal{K}^{\text{inv}}$ is some fixed purification. This can be proven by noting that any purification of ρ has the form (28); thus it is obtained by applying a local unitary $\mathbb{1} \otimes U_A$ to $|\Psi_0\rangle$. Therefore, $\mathcal{E}_\mathcal{H}^{\text{inv}}$ can be identified with the quotient manifold $\mathcal{S}_\mathcal{K}^{\text{inv}}/U(n_A)$ and π is the quotient map.

An important fact about π is that its differentials $d\pi|_{|\Psi\rangle} : T_{|\Psi\rangle} \mathcal{S}_\mathcal{K} \rightarrow T_\rho \mathcal{E}_\mathcal{H}$ are surjective for any $|\Psi\rangle \in \mathcal{S}_\mathcal{K}^{\text{inv}}$. Such quotient maps with surjective differentials are called smooth submersions. The differentials of the map (27) are given by

$$d\pi|_{|\Psi\rangle}(|\dot{\Psi}\rangle) = \text{tr}_A(|\Psi\rangle\langle\dot{\Psi}| + |\dot{\Psi}\rangle\langle\Psi|). \quad (33)$$

To prove that $\pi : \mathcal{S}_{\mathcal{K}}^{\text{inv}} \rightarrow \mathcal{E}_{\mathcal{H}}^{\text{inv}}$ is a smooth submersion, let us first note that for any fixed $\dot{\rho} \in T_{\rho}\mathcal{E}_{\mathcal{H}}$, if $|\dot{\Psi}\rangle \in \mathcal{K}$ satisfies

$$d\pi|_{|\Psi\rangle}(|\dot{\Psi}\rangle) = \dot{\rho} \quad (34)$$

then $|\dot{\Psi}\rangle \in T_{|\Psi\rangle}\mathcal{S}_{\mathcal{K}}$. In fact, by taking the trace of the right hand sides of (33) and (34) one gets $2\text{Re}\langle\Psi|\dot{\Psi}\rangle = \text{tr}\dot{\rho} = 0$. Setting $\rho = \pi(|\Psi\rangle)$, it is easy to check that $|\dot{\Psi}\rangle = \frac{1}{2}\dot{\rho}\rho^{-1} \otimes \mathbb{1}|\Psi\rangle$ is a solution of (34). Hence $d\pi|_{|\Psi\rangle}$ is surjective. Let us point out that this is not true if π is defined on the whole unit sphere $\mathcal{S}_{\mathcal{K}}$ of $\mathcal{K}$, instead of $\mathcal{S}_{\mathcal{K}}^{\text{inv}}$, i.e., if one adds to $\mathcal{E}_{\mathcal{H}}^{\text{inv}}$ its boundary $\partial\mathcal{E}_{\mathcal{H}}$.

3.3 Riemannian submersions

Our results in this paper rely on the notion of Riemannian submersion. In this subsection we review the properties of such submersions (see e.g. [33] for more details) and show that the partial trace (27) is an instance of Riemannian submersion $\mathcal{S}_{\mathcal{K}}^{\text{inv}} \rightarrow \mathcal{E}_{\mathcal{H}}^{\text{inv}}$.

Let $\pi : \mathcal{X} \rightarrow \mathcal{E}$ be a smooth submersion, where $\mathcal{X}$ is a Riemannian manifold with metric $g_{\mathcal{X}}$. The tangent space $T_{\psi}\mathcal{X}$ at $\psi \in \mathcal{X}$ can be decomposed into a direct sum of two orthogonal subspaces $\mathfrak{v}_{\psi} = \ker(d\pi|_{\psi})$ and $\mathfrak{h}_{\psi} = \mathfrak{v}_{\psi}^{\perp}$, called respectively the vertical and horizontal subspaces (orthogonality is for the scalar product $(g_{\mathcal{X}})_{\psi}$). It can be shown that there exists a unique Riemannian metric $g_{\mathcal{E}}$ on the quotient manifold $\mathcal{E}$ such that for all $\psi \in \mathcal{X}$, the restriction of $d\pi|_{\psi}$ to the horizontal subspace $\mathfrak{h}_{\psi}$ is an isometry from $(\mathfrak{h}_{\psi}, (g_{\mathcal{X}})_{\psi})$ to $(T_{\rho}\mathcal{E}, (g_{\mathcal{E}})_{\rho})$, with $\rho = \pi(\psi)$. One then says that $\pi : (\mathcal{X}, g_{\mathcal{X}}) \rightarrow (\mathcal{E}, g_{\mathcal{E}})$ is a Riemannian submersion. It is not difficult to prove that $g_{\mathcal{E}}$ is associated to the distance $d_{\mathcal{E}}$ on $\mathcal{E}$ defined by

$$d_{\mathcal{E}}(\rho, \sigma) = \inf_{\phi \in \pi^{-1}(\sigma)} d_{\mathcal{X}}(\psi_1, \phi), \quad (35)$$

where $d_{\mathcal{X}}$ is a distance having the metric $g_{\mathcal{X}}$ and ψ_1 is an arbitrary (fixed) point on the orbit of ρ .

A nice property of Riemannian submersions is that the geodesics on the quotient space $\mathcal{E}$ can be obtained by projecting certain geodesics on $\mathcal{X}$. More precisely, for any geodesic $\Gamma : [t_0, t_1] \rightarrow \mathcal{X}$ on $(\mathcal{X}, g_{\mathcal{X}})$ such that $\dot{\Gamma}(0) \in \mathfrak{h}_{\Gamma(0)}$, one has [33]:

- (i) $\dot{\Gamma}(t) \in \mathfrak{h}_{\Gamma(t)}$ for any $t \in [t_0, t_1]$;
- (ii) $\gamma = \pi \circ \Gamma$ is a geodesic on $(\mathcal{E}, g_{\mathcal{E}})$.

Conversely, any geodesic γ on $(\mathcal{E}, g_{\mathcal{E}})$ with $\gamma(0) = \rho$ can be lifted locally to a geodesic Γ on $(\mathcal{X}, g_{\mathcal{X}})$ with horizontal tangent vectors such that $\Gamma(0) = \psi$, for any $\psi \in \pi^{-1}(\rho)$. This property is illustrated in Fig. 1. We will call horizontal geodesics the geodesics Γ on $\mathcal{X}$ such that $\dot{\Gamma}(0) \in \mathfrak{h}_{\Gamma(0)}$.

Let us apply this formalism to the smooth submersion π given by (27). A natural distance on $\mathcal{S}_{\mathcal{K}}^{\text{inv}}$ having the euclidean metric $g_{\mathcal{S}}$ is the norm distance $d_{\mathcal{S}}(|\Psi\rangle, |\Phi\rangle) = \||\Psi\rangle - |\Phi\rangle\|$. The metric on $\mathcal{E}_{\mathcal{H}}^{\text{inv}}$

making π a Riemannian submersion turns out to be the Bures metric g_B . This can be seen by invoking Uhlmann's theorem, which states that [1, 2]

$$d_B(\rho, \sigma) = \min_{|\Psi\rangle \in \pi^{-1}(\rho), |\Phi\rangle \in \pi^{-1}(\sigma)} \arccos |\langle\Psi|\Phi\rangle|, \quad (36)$$

where in the right-hand side the arccos distance between pure states is minimized. Equivalently, the Bures distance $d_{\text{Bures}}(\rho, \sigma) = 2 \sin(d_B(\rho, \sigma)/2)$ is given by [4, 36]

$$\begin{aligned} d_{\text{Bures}}(\rho, \sigma) &= (2 - 2\sqrt{F(\rho, \sigma)})^{\frac{1}{2}} \\ &= \min_{|\Psi\rangle \in \pi^{-1}(\rho), |\Phi\rangle \in \pi^{-1}(\sigma)} \||\Psi\rangle - |\Phi\rangle\|. \end{aligned} \quad (37)$$

Note that the two distances d_B and d_{Bures} have the same metric g_B , given by (26). Eqs. (36) and (37) tell us that the arccos and Bures distances between ρ and σ are the minimal distances between the orbits of ρ and σ . By (32) and the unitary invariance of the scalar product in $\mathcal{K}$, the minima in these equations can be carried out over all $|\Phi\rangle \in \pi^{-1}(\sigma)$ for some fixed $|\Psi_1\rangle \in \pi^{-1}(\rho)$. Thus d_{Bures} has the form (35) with $d_{\mathcal{X}} = d_{\mathcal{S}}$.

3.4 Vertical and horizontal subspaces

Let us determine the vertical and horizontal subspaces in the case of the purification manifold $\mathcal{X} = \mathcal{S}_{\mathcal{K}}^{\text{inv}}$ and quotient map (27). To determine $\mathfrak{v}_{|\Psi\rangle} = \ker(d\pi|_{|\Psi\rangle})$, we observe that curves contained in the orbit $\pi^{-1}(\rho)$ have by definition vertical tangent vectors. Thus, denoting by $T_{|\Psi\rangle}\pi^{-1}(\rho)$ the tangent space of this orbit at $|\Psi\rangle$, it holds $T_{|\Psi\rangle}\pi^{-1}(\rho) \subset \mathfrak{v}_{|\Psi\rangle}$. To show that the inclusion is an equality, we now prove that the two subspaces have the same dimension. By the rank theorem and the surjectivity of $d\pi|_{|\Psi\rangle}$, one has

$$\begin{aligned} \dim_{\mathbb{R}}(\mathfrak{v}_{|\Psi\rangle}) &= \dim_{\mathbb{R}}(T_{|\Psi\rangle}\mathcal{S}_{\mathcal{K}}) - \dim_{\mathbb{R}}(T_{\rho}\mathcal{E}_{\mathcal{H}}) \\ &= (2nn_{\mathcal{A}} - 1) - (n^2 - 1) = n(2n_{\mathcal{A}} - n). \end{aligned} \quad (38)$$

On the other hand, by (28) and $\rho > 0$, purifications of ρ are in one-to-one correspondence with families $\{|\alpha_k\rangle\}_{k=1}^n$ of n orthonormal vectors in $\mathcal{H}_{\mathcal{A}}$. It is easy to show that these families form a manifold of real dimension $n(2n_{\mathcal{A}} - n)$. Hence $\mathfrak{v}_{|\Psi\rangle} = T_{|\Psi\rangle}\pi^{-1}(\rho)$. Thus, by (32) one has

$$\mathfrak{v}_{|\Psi\rangle} = \{\mathbb{1} \otimes K_{\mathcal{A}}|\Psi\rangle; K_{\mathcal{A}} \text{ skew Hermitian}\}. \quad (39)$$

We point out that (39) is incorrect for non-invertible states $\rho \in \partial\mathcal{E}_{\mathcal{H}}$. In fact, if $r = \text{rank}(\rho) < n$ then $\dim_{\mathbb{R}}(T_{|\Psi\rangle}\pi^{-1}(\rho)) = r(2n_{\mathcal{A}} - r)$ is strictly smaller than $\dim_{\mathbb{R}}(\mathfrak{v}_{|\Psi\rangle}) = 2n(n_{\mathcal{A}} - r) + r^2$.

In order to obtain the horizontal subspace $\mathfrak{h}_{|\Psi\rangle} = \mathfrak{v}_{|\Psi\rangle}^{\perp}$, we use the Schmidt decomposition (28) and expand an arbitrary horizontal tangent vector $|\dot{\Psi}^h\rangle = \sum_{k,l} c_{kl}|k\rangle|\alpha_l\rangle$ in the product basis $\{|k\rangle|\alpha_l\rangle\}_{k,l=1}^{n,n_{\mathcal{A}}}$.

Since $|\dot{\Psi}^h\rangle$ is orthogonal to $\mathfrak{h}_{|\Psi\rangle}$, one finds

$$\begin{aligned} 0 &= \text{Re} \langle \dot{\Psi}^h | \mathbb{1} \otimes K_A | \Psi \rangle \\ &= \sum_{k,l=1}^{n,n_A} (\bar{c}_{kl} \sqrt{p_k} \langle \alpha_l | K_A | \alpha_k \rangle - c_{kl} \sqrt{p_k} \langle \alpha_k | K_A | \alpha_l \rangle) \end{aligned} \quad (40)$$

for any skew Hermitian ancilla operator K_A . Choosing $K_A = i^\nu |\alpha_l\rangle\langle\alpha_k| - (-i)^\nu |\alpha_k\rangle\langle\alpha_l|$ with $\nu = 0$ or 1 , this gives

$$c_{kl} \sqrt{p_k} = \begin{cases} \bar{c}_{lk} \sqrt{p_l} & \text{if } 1 \leq k, l \leq n \\ 0 & \text{if } n < l \leq n_A. \end{cases} \quad (41)$$

Let us set $L_S = \sum_{k,l=1}^n \ell_{kl} |k\rangle\langle l|$ with $\ell_{kl} = c_{kl} p_l^{-\frac{1}{2}}$. It follows from (41) that $L_S = L_S^\dagger$. Furthermore,

$$|\dot{\Psi}^h\rangle = \sum_{k,l=1}^n \ell_{kl} \sqrt{p_l} |k\rangle |\alpha_l\rangle = L_S \otimes \mathbb{1}_A |\Psi\rangle. \quad (42)$$

Reciprocally, if $|\dot{\Psi}^h\rangle = L_S \otimes \mathbb{1}_A |\Psi\rangle$ with L_S self-adjoint then $\text{Re} \langle \dot{\Psi}^h | \mathbb{1} \otimes K_A | \Psi \rangle = 0$. The condition $\text{Re} \langle \dot{\Psi}^h | \Psi \rangle = 0$ coming from the requirement that $|\dot{\Psi}^h\rangle$ is in the tangent space (30) yields the additional constraint $\langle L_S \otimes \mathbb{1}_A \rangle_\Psi = 0$. Thus

$$\mathfrak{h}_{|\Psi\rangle} = \{L_S \otimes \mathbb{1}_A |\Psi\rangle; L_S \text{ self-adjoint}, \langle L_S \otimes \mathbb{1}_A \rangle_\Psi = 0\}. \quad (43)$$

In conclusion, we have shown that the partial trace map (27) defines a Riemannian submersion from $\mathcal{S}_{\mathcal{K}}^{\text{inv}}$ equipped with the metric g_S to the manifold $\mathcal{E}_{\mathcal{H}}^{\text{inv}}$ equipped with the Bures metric g_B . This means that $d\pi$ is an isometry from $(\mathfrak{h}_{|\Psi\rangle}, g_S)$ to $(T_\rho \mathcal{E}_{\mathcal{H}}, g_B)$, namely,

$$(g_B)_\rho (d\pi_{|\Psi\rangle}(|\dot{\Psi}^h\rangle), d\pi_{|\Psi\rangle}(|\dot{\Phi}^h\rangle)) = \text{Re} \langle \dot{\Psi}^h | \dot{\Phi}^h \rangle \quad (44)$$

for any purification $|\Psi\rangle$ of ρ and any horizontal tangent vectors $|\dot{\Psi}^h\rangle, |\dot{\Phi}^h\rangle \in \mathfrak{h}_{|\Psi\rangle}$.

4 Bures geodesics

4.1 Determination of the geodesics

We determine in this subsection the Bures geodesics by applying the mathematical framework of the preceding section (see [45] for a similar approach in the case of the space of positive definite matrices, i.e., unnormalized quantum states).

The shortest geodesic arc joining two vectors $|\Psi\rangle$ and $|\Phi\rangle$ on the unit sphere $\mathcal{S}_{\mathcal{K}}^{\text{inv}}$ equipped with the metric g_S is the arc of great circle

$$|\Psi_g(\tau)\rangle = \cos \tau |\Psi\rangle + \sin \tau |\dot{\Psi}\rangle, \quad 0 \leq \tau \leq \theta, \quad (45)$$

where $|\dot{\Psi}\rangle \in T_{|\Psi\rangle} \mathcal{S}_{\mathcal{K}}^{\text{inv}}$ and $\theta = \arccos(\text{Re} \langle \Psi | \Phi \rangle)$ is the angle between $|\Psi\rangle$ and $|\Phi\rangle$. We may assume without loss of generality that $\theta \neq 0, \pi$, since otherwise $|\Psi\rangle$ and $|\Phi\rangle = \pm |\Psi\rangle$ project out to the same state

$\rho = \sigma$. The longest arc of great circle joining $|\Psi\rangle$ and $|\Phi\rangle$ needs not be considered here, because it is the extension of the shortest geodesic joining $|\Psi\rangle$ and $-|\Phi\rangle$ and the latter vector belongs to the same orbit as $|\Phi\rangle$. The geodesic tangent vector at $\tau = 0$ is given by

$$|\dot{\Psi}_g(0)\rangle = |\dot{\Psi}\rangle = \frac{1}{\sin \theta} (|\Phi\rangle - \cos \theta |\Psi\rangle). \quad (46)$$

It is easy to check on this formula that $\|\dot{\Psi}\| = 1$, i.e., the geodesic (45) has unit velocity.

According to the properties of Riemannian submersions (Sec. 3.3), the Bures geodesic arcs joining the invertible states $\rho = \pi(|\Psi\rangle)$ and $\sigma = \pi(|\Phi\rangle)$ are obtained by projecting the arcs of great circle (45) having horizontal tangent vectors $|\dot{\Psi}\rangle \in \mathfrak{h}_\Psi$. Let us consider the purification of ρ given by

$$|\Psi\rangle = \sqrt{\rho} \otimes \mathbb{1}_A \sum_{k=1}^n |k\rangle |\alpha_k\rangle, \quad (47)$$

where we have used the Schmidt decomposition (28). The last sum is an (unnormalized) maximally entangled state of the system and ancilla. Similarly, by (32) any purification of σ has the form

$$|\Phi\rangle = \sqrt{\sigma} \rho^{-1/2} \otimes U_A |\Psi\rangle, \quad (48)$$

where U_A is a unitary on $\mathcal{H}_A$.

It is convenient at this point to introduce the polar decomposition

$$\sqrt{\sigma} \sqrt{\rho} = U_{\sigma\rho} \Lambda_{\sigma\rho}, \quad \Lambda_{\sigma\rho} = |\sqrt{\sigma} \sqrt{\rho}| > 0, \quad (49)$$

where $U_{\sigma\rho}$ is unitary.

We have to determine the purifications $|\Phi\rangle$ of σ such that the horizontality condition $|\dot{\Psi}\rangle \in \mathfrak{h}_{|\Psi\rangle}$ holds. We will show that:

Lemma 1. *The purifications of σ such that $|\dot{\Psi}\rangle \in \mathfrak{h}_{|\Psi\rangle}$ are given by*

$$|\Phi_V\rangle = M_{\rho\sigma,V} \otimes \mathbb{1}_A |\Psi\rangle \quad (50)$$

with

$$M_{\rho\sigma,V} = \sqrt{\sigma} U_{\sigma\rho} V \rho^{-1/2} = \rho^{-1/2} \Lambda_{\sigma\rho} V \rho^{-1/2}, \quad (51)$$

where V is an arbitrary unitary and self-adjoint operator commuting with $\Lambda_{\sigma\rho}$.

Proof. In view of (43), (46), (47), and (48), the horizontality condition can be written as

$$\begin{aligned} &\frac{1}{\sin \theta} \left(\sqrt{\sigma} \mathbb{1} \otimes U_A - \cos \theta \sqrt{\rho} \otimes \mathbb{1}_A \right) \sum_{k=1}^n |k\rangle |\alpha_k\rangle \\ &= L_S \sqrt{\rho} \otimes \mathbb{1}_A \sum_{k=1}^n |k\rangle |\alpha_k\rangle \end{aligned} \quad (52)$$

for some self-adjoint operator L_S such that $\langle L_S \otimes \mathbb{1}_A \rangle_\Psi = 0$. In particular, one has $\langle \alpha_l | U_A | \alpha_k \rangle = 0$ for $n < l \leq n_A$ and $1 \leq k \leq n$. We now use the identity

$$\mathbb{1} \otimes U_A \sum_{k=1}^n |k\rangle |\alpha_k\rangle = U_A^T \otimes \mathbb{1}_A \sum_{k=1}^n |k\rangle |\alpha_k\rangle, \quad (53)$$

where $U_A^T = \sum_{k,l=1}^n \langle \alpha_l | U_A | \alpha_k \rangle |k\rangle \langle l|$ (when $n_A > n$, (53) is true provided that $\text{span}\{|\alpha_1\rangle, \dots, |\alpha_n\rangle\}$ is invariant under U_A , which is indeed the case here). Observe that $U = U_A^T$ is unitary. Multiplying both members of (52) by $\sqrt{\rho}$, one deduces that this equation is equivalent to

$$\frac{1}{\sin \theta} \left(\sqrt{\rho} \sqrt{\sigma} U - \cos \theta \rho \right) = \sqrt{\rho} L_S \sqrt{\rho}. \quad (54)$$

Therefore, (52) is equivalent to $\sqrt{\rho} \sqrt{\sigma} U$ being self-adjoint for some unitary U on $\mathcal{H}$. (As we shall see below, this self-adjointness implies $\langle \Psi | \Phi \rangle \in \mathbb{R}$, thus $\langle \Psi | \dot{\Psi} \rangle = \text{Re} \langle \Psi | \dot{\Psi} \rangle = 0$ by (46) and $|\dot{\Psi}\rangle \in T_{|\Psi\rangle} \mathcal{S}_{\mathcal{K}}^{\text{inv}}$. Hence $\langle L_S \otimes \mathbb{1}_A \rangle_{\Psi} = 0$ does not yield an additional condition.)

Let V be the unitary operator given by $V = U_{\sigma\rho}^\dagger U$. Then by (49), $\sqrt{\rho} \sqrt{\sigma} U$ is self-adjoint if and only if $\Lambda_{\sigma\rho} V = V^\dagger \Lambda_{\sigma\rho}$. This implies $V^\dagger \Lambda_{\sigma\rho}^2 V = \Lambda_{\sigma\rho}^2$, i.e., V commutes with $\Lambda_{\sigma\rho}^2$ and thus with $\Lambda_{\sigma\rho}$. As a result, $V^\dagger \Lambda_{\sigma\rho} = V \Lambda_{\sigma\rho}$, which entails $V^\dagger = V$ (since $\Lambda_{\sigma\rho} > 0$). Thus the horizontality condition (52) holds if and only if $U = U_{\sigma\rho} V$ with V unitary, self-adjoint, and $[V, \Lambda_{\sigma\rho}] = 0$. The corresponding purifications of σ are given by (50). $\square$

Note that $\langle \Psi | \Phi_V \rangle$ is real. By (45) and (46), the horizontal geodesics on $\mathcal{S}_{\mathcal{K}}^{\text{inv}}$ are given by

$$|\Psi_{g,V}(\tau)\rangle = \frac{1}{\sin \theta_V} \left(\sin(\theta_V - \tau) |\Psi\rangle + \sin \tau |\Phi_V\rangle \right) \quad (55)$$

with $\cos \theta_V = \langle \Psi | \Phi_V \rangle = \text{tr} \Lambda_{\sigma\rho} V$.

By using the identity

$$\text{tr}_A |\Phi_V\rangle \langle \Psi| = \sqrt{\sigma} U_{\sigma\rho} V \sqrt{\rho} = \rho^{-1/2} \Lambda_{\sigma\rho} V \sqrt{\rho}, \quad (56)$$

we obtain the geodesics $\gamma_{g,V}(\tau) = \pi(|\Psi_{g,V}(\tau)\rangle)$ on $\mathcal{E}_{\mathcal{H}}$, where π is the quotient map (27),

$$\begin{aligned} \gamma_{g,V}(\tau) = & \frac{1}{\sin^2 \theta_V} \left(\sin^2(\theta_V - \tau) \rho + \sin^2(\tau) \sigma + \right. \\ & \left. + \sin(\theta_V - \tau) \sin \tau \left(\rho^{-1/2} \Lambda_{\sigma\rho} V \rho^{1/2} + \text{h.c.} \right) \right) \end{aligned} \quad (57)$$

with $0 \leq \tau \leq \theta_V$. Eq. (57) generalizes formula (1) of Sec. 2. It coincides with this formula for $V = \mathbb{1}$. Thanks to (44) and by the horizontality of $|\dot{\Psi}_V\rangle$, $\gamma_{g,V}$ has unit square velocity $(g_B)_\rho(\dot{\gamma}_{g,V}, \dot{\gamma}_{g,V}) = \|\dot{\Psi}_V\|^2 = 1$. Thus $\theta_V = \ell(\gamma_{g,V})$ is the geodesic length.

The geodesic with the smallest length is obtained for $V = \mathbb{1}$. In fact, for an arbitrary unitary and self-adjoint V commuting with $\Lambda_{\sigma\rho}$, denoting by $\lambda_k > 0$ and $v_k \in \{-1, 1\}$ the eigenvalues of $\Lambda_{\sigma\rho}$ and V , one has

$$\begin{aligned} \cos \theta_V = \text{tr} \Lambda_{\sigma\rho} V &= \sum_{k=1}^n \lambda_k v_k \\ &\leq \sum_{k=1}^n \lambda_k = \text{tr} \Lambda_{\sigma\rho} = \sqrt{F(\rho, \sigma)} = \cos \theta_1, \end{aligned} \quad (58)$$

where we have set $\theta_1 = \theta_{V=\mathbb{1}}$. Similarly, the longest geodesic joining ρ to σ is obtained by choosing $V = -\mathbb{1}$ and has length $\pi - \theta_1$. In view of (50), such a geodesic is the projection of the arc of great circle joining $|\Psi\rangle$ and the vector $|\Phi_{-1}\rangle = -|\Phi_1\rangle$ diametrically opposite to $|\Phi_1\rangle$ on the sphere $\mathcal{S}_{\mathcal{K}}^{\text{inv}}$. The latter is obtained by inverting time on the great circle through $|\Psi\rangle$ and $|\Phi_1\rangle$ and replacing the arc length θ_1 by $\pi - \theta_1$. Thus, by extending the shortest and longest geodesic arcs $\gamma_{g,1}$ and $\gamma_{g,-1}$ joining ρ and σ to the interval $[0, \pi]$, one obtains the same closed curve albeit with opposite orientations. More generally, the pair of geodesics $(\gamma_{g,V}, \gamma_{g,-V})$ enjoys the same property.

We have proven:

Theorem 1. *The Bures geodesic arcs joining the two distinct invertible states ρ and $\sigma \in \mathcal{E}_{\mathcal{H}}^{\text{inv}}$ are given by*

$$\gamma_{g,V}(\tau) = X_{\rho\sigma,V}(\tau) \rho X_{\rho\sigma,V}(\tau), \quad 0 \leq \tau \leq \theta_V, \quad (59)$$

where the geodesic length θ_V is given by (58) and $X_{\rho\sigma,V}(\tau)$ is the operator defined by

$$X_{\rho\sigma,V}(\tau) = \frac{1}{\sin \theta_V} \left(\sin(\tau) M_{\rho\sigma,V} + \sin(\theta_V - \tau) \mathbb{1} \right) \quad (60)$$

with $M_{\rho\sigma}$ given by (51). Here, V is an arbitrary unitary self-adjoint operator commuting with $\Lambda_{\sigma\rho} = |\sqrt{\sigma} \sqrt{\rho}|$. Furthermore, the geodesic with the smallest length, denoted hereafter by γ_g , is obtained by choosing $V = \mathbb{1}$ in (51), (59) and (60) and has length

$$\ell(\gamma_g) = \theta_1 = d_B(\rho, \sigma) \in (0, \frac{\pi}{2}]. \quad (61)$$

The explicit form (59) of the Bures geodesics have been obtained in Refs. [34, 35] in the special case $V = \mathbb{1}$. Our derivation shows that, in addition to this shortest geodesic, there are other geodesics having larger lengths θ_V , corresponding to $V \neq \mathbb{1}$. More precisely, there are 2^n geodesic arcs joining two invertible states ρ and σ if $\Lambda_{\sigma\rho}$ has a non-degenerate spectrum. In contrast, if $\Lambda_{\sigma\rho}$ has a degenerate eigenvalue λ_k there are infinitely many geodesics $\gamma_{g,V}$ joining ρ and σ , in analogy with what happens for diametrically opposite points on a sphere. Actually, in the non-degenerate case there are 2^n choices for V because V is diagonal in an eigenbasis of $\Lambda_{\sigma\rho}$ (since $[\Lambda_{\sigma\rho}, V] = 0$) and thus is fully characterized by its eigenvalues $v_k \in \{1, -1\}$. In the degenerate case, $V_k = \Pi_k V \Pi_k$ can be any $r_k \times r_k$ self-adjoint unitary matrix, where Π_k and r_k are the eigenprojector and multiplicity of λ_k , thus there are infinitely many choices for V . Note that in all cases there are at most 2^n distinct geodesic lengths $\theta_V = \ell(\gamma_{g,V})$ since θ_V only depends on the spectrum of V , see (58). The geodesic with the shortest length is always unique and obtained for $V = \mathbb{1}$. The second shortest geodesic length θ_2 is given by $\cos \theta_2 = \cos \theta_1 - 2\lambda_{\min}$, $\lambda_{\min}$ being the smallest eigenvalue of $\Lambda_{\sigma\rho}$. If $\lambda_{\min}$ is not degenerated, the corresponding geodesic is unique and

obtained by choosing $V = V_{i_m}$ such that it has a single negative eigenvalue $v_{i_m} = -1$, with $\lambda_{i_m} = \lambda_{\min}$.

One infers from (61) that the geodesic distance (obtained as the minimal length of curves joining ρ and σ) is the arccos Bures distance d_B , see (22). This is the main reason for working with that distance, instead of the Bures distance (37); $d_B(\rho, \sigma)$ is the angle $\theta_1 = \arccos\langle\Psi|\Phi_{\mathbb{1}}\rangle$ between the purification vectors $|\Psi\rangle$ and $|\Phi_{\mathbb{1}}\rangle$ of ρ and σ (recall that $\langle\Psi|\Phi_V\rangle \in \mathbb{R}$). Hence $|\Phi\rangle = |\Phi_{\mathbb{1}}\rangle$ (and similarly $|\Phi_{-\mathbb{1}}\rangle = -|\Phi_{\mathbb{1}}\rangle$) is a purification of σ maximizing the pure state fidelity $|\langle\Psi|\Phi\rangle|$ in Uhlmann's theorem $\sqrt{F(\rho, \sigma)} = \max_{|\Phi\rangle} |\langle\Psi|\Phi\rangle|$ [1, 2]. This gives a way to compute $|\Phi_{\mathbb{1}}\rangle$ numerically using an optimization algorithm, instead of relying on the formula (50) (note that to compute $|\Phi_{\mathbb{1}}\rangle$ from (50) one needs to diagonalize ρ and $\sqrt{\sigma}\sqrt{\rho}$). The purifications $|\Phi_V\rangle$ for $V \neq \pm\mathbb{1}$ correspond to relative maxima of $|\langle\Psi|\Phi\rangle|$, which are smaller than the global maximum, see (58).

The properties of the self-adjoint operators (51) are given in Appendix A. As pointed out in [34], for $V = \mathbb{1}$, $M_{\rho\sigma, \mathbb{1}}$ is related to the optimal measurement to discriminate the distributions of measurement outcomes in states ρ and σ (more precisely, the Hellinger distance between these two distributions is maximum for a projective measurement in the eigenbasis of $M_{\rho\sigma, \mathbb{1}}$ [4]).

4.2 Geodesics joining commuting states

In the special case of commuting states ρ and σ , the geodesics have the form

$$\gamma_{g,V}(\tau) = \sum_k p_{k,V}(\tau) |k\rangle\langle k| \quad (62)$$

$$p_{k,V}(\tau) = \left(\frac{\sin(\theta_V - \tau)}{\sin \theta_V} \sqrt{p_k} + v_k \frac{\sin \tau}{\sin \theta_V} \sqrt{q_k} \right)^2,$$

where $\{|k\rangle\}$ is an orthonormal basis of common eigenvectors of ρ and σ and p_k, q_k are the corresponding eigenvalues. In fact, then $M_{\rho\sigma, V} = \sum_k v_k \sqrt{q_k/p_k} |k\rangle\langle k|$ and the purification (50) of σ is given by

$$|\Phi_V\rangle = \sum_k v_k \sqrt{q_k} |k\rangle |\alpha_k\rangle_A. \quad (63)$$

Replacing this expression into (55) yields the horizontal geodesic $|\Psi_{g,V}\rangle(\tau) = \sum_k \sqrt{p_{k,V}(\tau)} |k\rangle |\alpha_k\rangle_A$, showing that $\gamma_{g,V}(\tau)$ commutes with ρ and σ at all times and is given by (62). Here, we have assumed that $\Lambda_{\sigma\rho}$ has a non-degenerated spectrum, i.e., $p_k q_k \neq p_l q_l$ if $k \neq l$. Otherwise, there are infinitely many geodesics from ρ to σ , which are not diagonal in the $\{|k\rangle\}$ -basis save for the one given by (62).

The quantum circuit of Fig. 2(a) with the unitary U_{SA} of Fig. 2(b) implements a geodesic joining commuting states. Indeed, using $|\Psi\rangle = \sum_k \sqrt{p_k} |w_k\rangle |k\rangle_A$ and $|\dot{\Psi}\rangle = U_{SA}|1\rangle|0\rangle_A = \sum_k \alpha_k |w_k\rangle |k\rangle_A$ one finds

that $|\Phi_V\rangle$ has the form (63) with $|k\rangle \hookrightarrow |w_k\rangle$ and $|\alpha_k\rangle_A \hookrightarrow |k\rangle_A$.

4.3 Intersections with the boundary of quantum states

We have so far determined the geodesics on the open manifold $\mathcal{E}_{\mathcal{H}}^{\text{inv}}$ but have not discussed whether such geodesics can bounce on its boundary $\partial\mathcal{E}_{\mathcal{H}}$. Let us consider the extension of the geodesic arc (59) joining the two states ρ and σ to the time interval $[0, \pi]$. This extension is a closed curve, which we still denote by $\gamma_{g,V}$. Generalizing a result obtained in [34], we show in Appendix B that this curve intersects q_V times the boundary, where q_V is the number of distinct eigenvalues of the observable $M_{\rho\sigma, V}$ in (51). More precisely, let ρ_i , $i = 1, \dots, q_V$, be the intersection points of $\gamma_{g,V}$ with $\partial\mathcal{E}_{\mathcal{H}}$. Theorem 6 in Appendix B shows that the states ρ_i have ranks $n - m_{i,V}$ and supports $(\mathbb{1} - P_{i,V})\mathcal{H}$, where $m_{i,V}$ and $P_{i,V}$ are the multiplicity and spectral projector of the i th eigenvalue of $M_{\rho\sigma, V}$. As a result, $\sum_{i=1}^{q_V} \dim(\ker(\rho_i)) = n$. In particular, $\gamma_{g,V}$ intersects $\partial\mathcal{E}_{\mathcal{H}}$ at a pure state if and only if the spectrum of $M_{\rho\sigma, V}$ has $q_V = 2$ eigenvalues. An interpretation of the states ρ_i and their kernel $P_{i,V}\mathcal{H}$ in quantum metrology is given in Sec 6.3 below.

Furthermore, it is shown in Appendix B that the number of intersections on the part of $\gamma_{g,V}$ joining ρ and σ is equal to the multiplicity of the eigenvalue -1 of V . In particular, the shortest geodesic γ_g does not intersect $\partial\mathcal{E}_{\mathcal{H}}$ between ρ and σ , while all other geodesics with $V \neq \mathbb{1}$ do so at least once.

4.4 Geodesics passing through a pure state

Consider an invertible state $\rho > 0$ and a pure state $\rho_1 = |\phi_1\rangle\langle\phi_1|$ such that $\langle\rho|\phi_1\rangle = \langle\phi_1|\rho|\phi_1\rangle > 0$. As shown in Theorem 6, there is up to time reversal only one geodesic joining ρ and ρ_1 . This geodesic is given by

$$\gamma_{g,\rho \rightarrow \rho_1}(\tau) = \frac{1}{\sin^2 \theta_1} \left(\sin^2(\theta_1 - \tau) \rho + \sin^2(\tau) \times |\phi_1\rangle\langle\phi_1| + \frac{\sin(\theta_1 - \tau) \sin(\tau)}{\cos \theta_1} \{ \rho, |\phi_1\rangle\langle\phi_1| \} \right) \quad (64)$$

with $\theta_1 = \arccos(\langle\rho|\phi_1\rangle^{1/2})$. This geodesic intersects twice the boundary, at ρ_1 and at another state ρ_2 of rank $n - 1$ and support orthogonal to $|\phi_1\rangle$. Eq. (64) can be proven from (57) by taking $\sigma = (1 - \varepsilon)\rho_1 + (\varepsilon/n)\mathbb{1} > 0$ and letting $\varepsilon \rightarrow 0$.

If $|\phi_1\rangle$ is an eigenvector of ρ with eigenvalue $p_1 = \cos^2(\theta_1) > 0$ then $\gamma_{g,\rho \rightarrow \rho_1}$ is a segment of straight line. In fact, in that case (64) simplifies to

$$\gamma_{g,\rho \rightarrow \rho_1}(\tau) = \sin^2(\theta_1 - \tau) \rho_{\perp} + \cos^2(\theta_1 - \tau) |\phi_1\rangle\langle\phi_1|, \quad (65)$$

where $\rho_{\perp} = \Pi_{\perp} \rho \Pi_{\perp} / \sin^2(\theta_1)$ and $\Pi_{\perp} = \mathbb{1} - |\phi_1\rangle\langle\phi_1|$ is the projector onto the subspace orthogonal to $|\phi_1\rangle$.

Note that this agrees with the general form (62) of geodesics between commuting states. Recall that the closest pure state to ρ , i.e., the state $|\phi_1\rangle$ maximizing the fidelity $F(\rho, \rho_1) = \langle \rho | \phi_1 \rangle$, is an eigenvector of ρ associated to the maximal eigenvalue. Hence the shortest path joining ρ to its closest pure state is a segment of straight line intersecting $\partial\mathcal{E}_{\mathcal{H}}$ transversally.

5 Geodesics as physical evolutions

We show in this section that the Bures geodesics correspond to physical evolutions of the system coupled to an ancilla and that such evolutions are non-Markovian.

Let us recall that the dynamics of an open quantum system coupled to its environment is obtained by letting the total system (system and environment) evolve unitarily under some Hamiltonian H and then tracing out over the environment (referred to as the ancilla A in what follows). The system state at time $t \geq 0$ is given by

$$\rho(t) = \text{tr}_A e^{-itH} |\Psi\rangle\langle\Psi| e^{itH}, \quad (66)$$

where $|\Psi\rangle$ is the system–ancilla initial state. Although one usually assumes that the system starts interacting with the ancilla at $t = 0$, so that $|\Psi\rangle = |\psi\rangle|\alpha\rangle$ is a product state, in general the two subsystems can be initially entangled.

We have seen in Sec. 4.1 that the Bures geodesics $\gamma_{g,V}(\tau)$ joining two states ρ and $\sigma \in \mathcal{E}_{\mathcal{H}}^{\text{inv}}$ are the projection of horizontal pure–state geodesics $|\Psi_{g,V}(\tau)\rangle$ on an enlarged system with Hilbert space $\mathcal{K} = \mathcal{H} \otimes \mathcal{H}_A$, i.e.,

$$\gamma_{g,V}(\tau) = \text{tr}_A |\Psi_{g,V}(\tau)\rangle\langle\Psi_{g,V}(\tau)|, \quad (67)$$

where $|\Psi_{g,V}(\tau)\rangle$ is given by (55). The following theorem shows that one can associate a Hamiltonian to the latter geodesic.

Theorem 2. *Consider the system-ancilla Hamiltonian*

$$\begin{aligned} H_{g,V} &= -i(|\Psi\rangle\langle\dot{\Psi}_V| - |\dot{\Psi}_V\rangle\langle\Psi|) \\ &= \frac{-i}{\sin\theta}(|\Psi\rangle\langle\Phi_V| - |\Phi_V\rangle\langle\Psi|), \end{aligned} \quad (68)$$

where $|\Psi\rangle \in \mathcal{K}$ is a fixed purification of ρ , $|\dot{\Psi}_V\rangle$ is the horizontal tangent vector to $|\Psi_{g,V}(\tau)\rangle$ at $\tau = 0$, and $|\Phi_V\rangle \in \mathcal{K}$ is the corresponding purification of σ , see (50). Then

$$|\Psi_{g,V}(\tau)\rangle = e^{-i\tau H_{g,V}} |\Psi\rangle \quad (69)$$

for any $\tau \geq 0$. As a result, the geodesic $\gamma_{g,V}$ coincides with the open quantum system time evolution

$$\gamma_{g,V}(\tau) = \text{tr}_A e^{-i\tau H_{g,V}} |\Psi\rangle\langle\Psi| e^{i\tau H_{g,V}}. \quad (70)$$

Proof. The horizontality condition $|\dot{\Psi}_V\rangle \in \mathfrak{h}_{|\Psi\rangle}$ entails $\langle\Psi|\dot{\Psi}_V\rangle = 0$, see (43) (note that general tangent vectors $|\dot{\Psi}\rangle$ at $|\Psi\rangle$ satisfy a weaker condition $\text{Re}\langle\Psi|\dot{\Psi}\rangle = 0$). Furthermore, one has $\|\dot{\Psi}_V\| = 1$, see the statement following (46). Let $\{|\Psi_k\rangle\}_{k=0}^{n_A-1}$ be an orthonormal basis of $\mathcal{K}$ such that $|\Psi_0\rangle = |\Psi\rangle$ and $|\Psi_1\rangle = |\dot{\Psi}_V\rangle$. The matrix of $H_{g,V}$ in this basis has a left upper corner given by the Pauli matrix σ_y , the other matrix elements being equal to zero. Such a matrix is easy to exponentiate, yielding

$$\begin{aligned} e^{-i\tau H_{g,V}} &= \mathbb{1} + (\cos\tau - 1)(|\Psi\rangle\langle\Psi| + |\dot{\Psi}_V\rangle\langle\dot{\Psi}_V|) \\ &\quad - \sin\tau(|\Psi\rangle\langle\dot{\Psi}_V| - |\dot{\Psi}_V\rangle\langle\Psi|). \end{aligned} \quad (71)$$

Applying this operator to $|\Psi\rangle$ and comparing with (45) yields the identity (69). The second equality in (68) follows from the relation (46) between $|\dot{\Psi}_V\rangle$ and $|\Phi_V\rangle$. $\square$

Note that the Hamiltonian $H_{g,V}$ does not depend on the choice of the initial state $|\Psi\rangle$ on the horizontal geodesic $|\Psi_{g,V}(\tau)\rangle$. Actually, let us fix another state $|\Psi_1\rangle = |\Psi_{g,V}(\tau_1)\rangle = \cos\tau_1|\Psi\rangle + \sin\tau_1|\dot{\Psi}_V\rangle$ on this geodesic. Since $|\Psi_{g,V}(0)\rangle \in \mathfrak{h}_{|\Psi\rangle}$, by property (i) of Sec. 3.3 the tangent vector $|\dot{\Psi}_{g,V}(\tau_1)\rangle = -\sin\tau_1|\Psi\rangle + \cos\tau_1|\dot{\Psi}_V\rangle$ is in the horizontal subspace at $|\Psi_1\rangle$. One easily checks that the expression of $H_{g,V}$ in the first line of (68) is invariant under the substitutions $|\Psi\rangle \leftrightarrow |\Psi_1\rangle$ and $|\dot{\Psi}_V\rangle \leftrightarrow |\dot{\Psi}_{g,V}(\tau_1)\rangle$.

The geodesics $\gamma_{g,V}$ in Theorem 1 depend on two invertible states ρ and σ . The purifications $|\Psi\rangle \in \mathcal{K}$ of ρ are entangled system-ancilla states. However, since one can choose any initial state on the geodesic, ρ can be taken to lie on the boundary $\partial\mathcal{E}_{\mathcal{H}}$ of quantum states. Recall that all geodesics intersect $\partial\mathcal{E}_{\mathcal{H}}$, see Sec. 4.3. Let us discuss the special case for which $\gamma_{g,V}$ has an intersection with $\partial\mathcal{E}_{\mathcal{H}}$ given by a pure state. For instance, all geodesics of a qubit satisfy this hypothesis (since $\partial\mathcal{E}_{\mathbb{C}^2}$ is the set of pure qubit states). One may then choose the initial state ρ on $\gamma_{g,V}$ to be a pure state $\rho_\psi = |\psi\rangle\langle\psi|$ having purifications $|\Psi\rangle = |\psi\rangle|\alpha\rangle$ given by product states, where $|\alpha\rangle$ is an arbitrary ancilla pure state. This means that the system and ancilla are initially uncorrelated. In that case one can extend the quantum evolution (70) to arbitrary (pure or mixed) initial states $\nu_S \in \mathcal{E}_{\mathcal{H}}$ of the system, by defining

$$\mathcal{M}_{g,V,\tau}(\nu_S) = \text{tr}_A e^{-i\tau H_{g,V}} \nu_S \otimes |\alpha\rangle\langle\alpha| e^{i\tau H_{g,V}}. \quad (72)$$

For all times τ , $\mathcal{M}_{g,V,\tau}$ is a quantum channel (CPTP map). The geodesic $\gamma_{g,V}(\tau) = \mathcal{M}_{g,V,\tau}(\rho_\psi)$ is obtained by taking the initial state $\nu_S = \rho_\psi$.

It is clear from (71) that the system-ancilla evolution operator $e^{-i\tau H_{g,V}}$ is periodic in time with period 2π . Thus the quantum evolution $\{\mathcal{M}_{g,V,\tau}\}_{\tau \geq 0}$ is also periodic; more precisely, it satisfies (6). As a consequence, this evolution is strongly non-Markovian. A quantitative study of this non-markovianity and a

Kraus decomposition of $\mathcal{M}_{g,V,\tau}$ will be presented in a forthcoming paper [43].

In conclusion, the Bures geodesics are not only mathematical objects but correspond to evolutions of the system coupled to an ancilla. This opens the route to the simulation of these geodesics on quantum computers and to their experimental observation. Examples of quantum circuits simulating some geodesics have been given above (see Fig. 2).

6 Geodesics in quantum metrology

In this section we study quantum parameter estimation for a quantum system coupled to an ancilla when measurements are not possible on the ancilla. We show that the Bures geodesics features optimal state transformations for estimating a parameter in a such situation.

6.1 Quantum Fisher information and Bures metric

As explained in Sec. 2.3, the best precision in the estimation of an unknown parameter x using quantum probes in output states ρ_x is given by the inverse square root of the QFI, see (10). The latter is by definition the maximum over all POVMs $\{M_j\}$ of the CFI (11) with probabilities $p_{j|x} = \text{tr} M_j \rho_x$. It is given by [39, 40]

$$\mathcal{F}_Q(x, \{\rho_x\}_{x \in X}) = \text{tr}[\rho_x L_x^2], \quad (73)$$

where L_x is a self-adjoint operator satisfying

$$\frac{1}{2}\{L_x, \rho_x\} = \dot{\rho}_x \quad (74)$$

with $\dot{\rho}_x = \partial_x \rho_x$. The operator L_x is called the symmetric logarithmic derivative of ρ_x . A POVM $\{M_j\}$ maximizes the CFI (i.e., $\mathcal{F}_{\text{clas}}(x, \{p_{j|x}\})_{x \in X} = \mathcal{F}_Q(x, \{\rho_x\}_{x \in X})$) if and only if $M_j^{1/2} \rho_x^{1/2}$ is equal to $c_j M_j^{1/2} L_x \rho_x^{1/2}$ for any j , with $c_j \in \mathbb{R}$ [40]. If ρ_x is invertible, this is equivalent to $M_j^{1/2} = c_j L_x M_j^{1/2}$. Thus, the optimal POVMs $\{M_j^{\text{opt}}\}$ maximizing the CFI are such that for any j , the support of M_j^{opt} is contained in an eigenspace of L_x . In particular, the projective measurement given by the spectral projectors of L_x is optimal. In general, the optimal measurements $\{M_j^{\text{opt}}\}$ depend on the estimated parameter x , as L_x depends on x .

It is known that for invertible states $\rho_x \in \mathcal{E}_{\mathcal{H}}^{\text{inv}}$ the QFI is equal to the Bures metric (26) up to a factor of four [4, 40],

$$\mathcal{F}_Q(x, \{\rho_x\}_{x \in X}) = 4(g_B)_{\rho_x}(\dot{\rho}_x, \dot{\rho}_x). \quad (75)$$

A similar relation holds for the CFI and the Fisher metric (see e.g. [41]). A way to derive the identity (75)

is as follows. Consider the geodesic $\gamma_{g,V}(\tau)$ passing through ρ_x at $\tau = 0$ with tangent vector $\dot{\gamma}_{g,V}(0) = \dot{\rho}_x$. By (67), one has

$$\dot{\rho}_x = \text{tr}_A(|\dot{\Psi}_{g,V}\rangle\langle\Psi_{g,V}| + |\Psi_{g,V}\rangle\langle\dot{\Psi}_{g,V}|) = \{L_S, \rho_x\}, \quad (76)$$

where the last equality comes from the horizontality condition $|\dot{\Psi}_{g,V}\rangle = L_S \otimes \mathbb{1}_A |\Psi_{g,V}\rangle$, see (4). Comparing with (74), one sees that the self-adjoint operator L_S is nothing but the symmetric logarithmic derivative L_x of ρ_x up to a factor of 1/2. Using the isometry property (44) of the metric, one gets

$$\begin{aligned} 4(g_B)_{\rho_x}(\dot{\rho}_x, \dot{\rho}_x) &= 4\|\dot{\Psi}_{g,V}\|^2 \\ &= \text{tr}(L_x \otimes \mathbb{1}_A |\Psi_{g,V}\rangle\langle\Psi_{g,V}| L_x \otimes \mathbb{1}_A) \\ &= \text{tr}(\rho_x L_x^2) = \mathcal{F}_Q(x, \{\rho_x\}_{x \in X}). \end{aligned} \quad (77)$$

We point out that the right-hand sides of (73) and (75) are not always equal for non-invertible states ρ_x . In fact, it is easy to show that the trace in (73) is given (up to a factor of four) by the right-hand side of (26) with $\dot{\sigma} = \dot{\rho}$ and a sum running over all indices k, l such that $p_k + p_l > 0$. On the other hand, as shown in [46], the Bures metric (which is defined in terms of the infinitesimal distance ds^2 , see (21)) is given by the same expression plus an additional term $2 \sum_{j, p_{j|x}=0} \partial_x^2 p_{j|x}$ involving the second derivatives of the vanishing eigenvalues of ρ_x (note that this term is absent when $\rho_x > 0$). As a result, the QFI (73) is discontinuous at values x at which $\text{rank}(\rho_x)$ is discontinuous, while the Bures metric remains continuous [42, 46]. This can be illustrated by the following example. Let $\rho_x = \sum_j p_{j|x} |j\rangle\langle j|$ with $\{|j\rangle\}$ a fixed orthonormal basis. Then the QFI (73) equals the CFI (11) and has a jump for trajectories $x \mapsto \rho_x$ bouncing on $\partial\mathcal{E}_{\mathcal{H}}$ at $x = x_0$. More precisely, each eigenvalue with a minimum at x_0 such that $p_{j|x_0} = \partial_x p_{j|x}(x_0) = 0$ contributes to the jump amplitude by $-\lim_{x \rightarrow x_0} (\partial_x p_{j|x})^2 / p_{j|x} = -2\partial_x^2 p_{j|x}(x_0)$. In contrast, $(g_B)_{\rho_x}(\dot{\rho}_x, \dot{\rho}_x)$ is continuous at x_0 due to aforementioned additional term canceling the discontinuity.

6.2 Pythagorean theorem and variational formula for the QFI

According to Stinespring's theorem [38], the action of an arbitrary quantum channel $\mathcal{M}_x$ on a state ρ_{in} can be obtained by coupling the system to an ancilla and letting the composite system evolving unitarily, assuming an initial system-ancilla product state $\rho_{\text{in}} \otimes |\alpha_0\rangle\langle\alpha_0|$. We suppose in what follows that this composite system is in a pure state $|\Psi_x\rangle$ undergoing a x -dependent unitary evolution of the form

$$|\Psi_x\rangle = e^{-ixH} |\Psi_{\text{in}}\rangle, \quad (78)$$

where H is some x -independent Hamiltonian on $\mathcal{K} = \mathcal{H} \otimes \mathcal{H}_A$ and the input system-ancilla state $|\Psi_{\text{in}}\rangle$ may

be entangled or not. The output states of the system are given by

$$\rho_x = \mathcal{M}_x(\rho_{\text{in}}) = \text{tr}_A |\Psi_x\rangle\langle\Psi_x|. \quad (79)$$

For concreteness, we assume that x belongs to an interval X containing 0. It is also convenient to replace H by $\Delta H = H - \langle H \rangle_{\Psi_{\text{in}}} \mathbb{1}$ in (78). This amounts to multiply $|\Psi_x\rangle$ by an irrelevant phase factor $e^{ix\langle H \rangle_{\Psi_{\text{in}}}}$. The QFI of the composite system reads (see (12))

$$\mathcal{F}_Q(\{|\Psi_x\rangle\}_{x \in X}) = 4\|\dot{\Psi}_x\|^2 = 4\langle(\Delta H)^2\rangle_{\Psi_{\text{in}}}, \quad (80)$$

where we have used that $\langle(\Delta H)^2\rangle_{\Psi_x}$ is independent of x .

As explained in Sec. 2.3, one can decompose the tangent vector $|\dot{\Psi}_x\rangle$ into its horizontal and vertical parts,

$$|\dot{\Psi}_x\rangle = -i\Delta H|\Psi_x\rangle = |\dot{\Psi}_x^h\rangle - i\mathbb{1} \otimes B_x^h|\Psi_x\rangle \quad (81)$$

with $|\dot{\Psi}_x^h\rangle \in \mathfrak{h}_{|\Psi_x\rangle}$ and B_x^h a self-adjoint operator on $\mathcal{H}_A$. Here, we have used the form (39) of the vertical subspace $\mathfrak{v}_{|\Psi_x\rangle}$. Note that $\langle \mathbb{1} \otimes B_x^h \rangle_{\Psi_x} = 0$ since $\langle \Psi_x | \dot{\Psi}_x \rangle = \langle \Psi_x | \dot{\Psi}_x^h \rangle = 0$. As $\rho_x = \pi(|\Psi_x\rangle)$ and $\mathfrak{v}_{|\Psi\rangle} = \ker(d\pi|_{|\Psi_x\rangle})$, where π is the projection (27), one has $\dot{\rho}_x = d\pi|_{|\Psi_x\rangle}(|\dot{\Psi}_x^h\rangle)$. Thanks to (44) and (75), the QFI is given by

$$\begin{aligned} \mathcal{F}_Q(x, \{\rho_x\}_{x \in X}) &= 4(g_B)_{\rho_x}(d\pi|_{|\Psi_x\rangle}(|\dot{\Psi}_x^h\rangle), d\pi|_{|\Psi_x\rangle}(|\dot{\Psi}_x^h\rangle)) \\ &= 4\|\dot{\Psi}_x^h\|^2 \\ &= 4(\|\dot{\Psi}_x\|^2 - \|\mathbb{1} \otimes B_x^h|\Psi_x\rangle\|^2), \end{aligned} \quad (82)$$

where the third equality follows from (81), the orthogonality of the horizontal and vertical subspaces, and the Pythagorean theorem. Using (80), one sees that (82) is equivalent to the formula (19) of Sec. 2.3. The skew Hermitian operator iB_x^h in (82) is the Uhlmann connection for the lift $x \in X \mapsto |\Psi_x\rangle$ of the curve $x \mapsto \rho_x$ [36].

It is instructive to derive from (82) the variational formula for the QFI from Ref. [26]. Consider the family of purifications of the ρ_y given by $|\tilde{\Psi}_y\rangle = \mathbb{1} \otimes e^{i(y-x)B_x}|\Psi_y\rangle$, where B_x is a self-adjoint operator on $\mathcal{H}_A$. Its tangent vector at $y = x$ is $\partial_y|\tilde{\Psi}_y\rangle|_x = |\dot{\Psi}_x\rangle + i\mathbb{1} \otimes B_x|\Psi_x\rangle = -i(\Delta H - \mathbb{1} \otimes B_x)|\Psi_x\rangle$. From (81) and Pythagorean theorem again, the square norm of this tangent vector is

$$\begin{aligned} \langle(\Delta H - \mathbb{1} \otimes B_x)^2\rangle_{\Psi_x} &= \|\dot{\Psi}_x^h\|^2 + \|\mathbb{1} \otimes (B_x - B_x^h)|\Psi_x\rangle\|^2 \\ &\geq \|\dot{\Psi}_x^h\|^2. \end{aligned} \quad (83)$$

Hence the minimum of the left-hand side over all B_x 's is equal to $\|\dot{\Psi}_x^h\|^2$ and the minimum is achieved for $B_x = B_x^h$. One deduces from (82) that [26]

$$\mathcal{F}_Q(x, \{\rho_x\}_{x \in X}) = 4 \min_{B_x = B_x^h} \langle(\Delta H - \mathbb{1} \otimes B_x)^2\rangle_{\Psi_x}. \quad (84)$$

Eq. (82) tells us that the QFI of the system is equal to the QFI (80) of the composite system minus a non-negative quantity $4\|\mathbb{1} \otimes B_x^h|\Psi_x\rangle\|^2$ that can be interpreted as the amount of information on x in the ancilla. Eq. (84) provides a variational formula for the QFI. Both expressions (82) and (84) have been derived in [26] by using another method. We see here that they have nice geometrical interpretations in the framework of Riemannian submersions, being simple consequences of the Pythagorean theorem.

6.3 Optimal precision in parameter estimation in open quantum systems

One deduces from (80) and (82) that the QFI of the probe is equal to the QFI of the composite system when the tangent vector $|\dot{\Psi}_x\rangle$ is horizontal (i.e., $B_x^h = 0$). In such a case, there is no information loss on the parameter x in the ancilla: joint measurements on the probe and ancilla do not lead to a better precision in the estimation than local measurements on the probe. However, in general the state transformation does not preserve the horizontality of the tangent vector. Let us assume for instance that $|\dot{\Psi}_{\text{in}}\rangle \in \mathfrak{h}_{|\Psi_{\text{in}}\rangle}$, so that the probe QFI is equal to $4\langle(\Delta H)^2\rangle_{\Psi_{\text{in}}}$ for $x = 0$. While the QFI of the composite system remains the same for all values of x , the probe QFI (82) depends on x and is strictly smaller than $4\langle(\Delta H)^2\rangle_{\Psi_{\text{in}}}$ for nonzero values of x at which $|\dot{\Psi}_x\rangle \notin \mathfrak{h}_{|\Psi_x\rangle}$, implying a larger error $(\Delta x)_{\text{QCRB}}$ for $x \neq 0$ than for $x = 0$. It is thus of interest to study situations for which the tangent vector remains horizontal for all values of the parameter. In such cases, the minimal error $(\Delta x)_{\text{QCRB}}$ is x -independent and equal to the minimal error one would obtain from joint measurements on the probe and ancilla.

In the following, we assume that both the system-ancilla coupling Hamiltonian H and the input state $|\Psi_{\text{in}}\rangle$ can be engineered at will. We look for Hamiltonians H and input states $|\Psi_{\text{in}}\rangle$ satisfying:

- (I) the horizontality condition $|\dot{\Psi}_x\rangle \in \mathfrak{h}_{|\Psi_x\rangle}$ holds for all $x \in X$;
- (II) for a fixed Hamiltonian H satisfying (I), $\|\dot{\Psi}_x\|^2 = \langle(\Delta H)^2\rangle_{\Psi_{\text{in}}}$ is maximum.

If conditions (I) and (II) are satisfied then the QFI of the system is constant and maximal for all values of x ,

$$\mathcal{F}_Q(x, \{\rho_x\}_{x \in X}) = 4\langle(\Delta H)^2\rangle_{\Psi_{\text{in}}}. \quad (85)$$

We shall assume that the highest and smallest eigenvalues of H , ϵ_{max} and ϵ_{min} , are non-degenerated. We set

$$\epsilon = \frac{1}{2}(\epsilon_{\text{max}} - \epsilon_{\text{min}}). \quad (86)$$

Our first result is:

Theorem 3. *Conditions (I) and (II) are fulfilled if and only if $|\dot{\Psi}_{\text{in}}\rangle = -i\Delta H|\Psi_{\text{in}}\rangle \in \mathfrak{h}_{|\Psi_{\text{in}}\rangle}$ and one of the two equivalent conditions holds*

$$(a) \quad |\Psi_x\rangle = e^{-ix\epsilon H_{g,V}} |\Psi_{\text{in}}\rangle, \quad x \in X;$$

$$(b) \quad \Pi(\Delta H)\Pi = \epsilon H_{g,V},$$

where $H_{g,V}$ is the geodesic Hamiltonian (3) with $|\Psi\rangle$ and $|\dot{\Psi}\rangle$ replaced by $|\Psi_{\text{in}}\rangle$ and $|\dot{\Psi}_{\text{in}}\rangle/\|\dot{\Psi}_{\text{in}}\|$, respectively, and Π is the projector onto the sum of the eigenspaces of H with eigenvalues ϵ_{max} and ϵ_{min} . Note that (a) implies

$$\rho_x = \gamma_{g,V}(x\epsilon), \quad x \in X \quad (87)$$

where $\gamma_{g,V}$ is a geodesic starting at the state $\rho_{\text{in}} = \text{tr}_A |\Psi_{\text{in}}\rangle\langle\Psi_{\text{in}}|$.

This theorem tells us that among all probe-ancilla Hamiltonians H having a fixed energy gap 2ϵ and assuming that the input state $|\Psi_{\text{in}}\rangle$ maximizes the probe-ancilla QFI for H , the Hamiltonians H producing the highest QFI of the probe, for arbitrary parameter values x , satisfy property (b), i.e., they generate geodesic evolutions given by (87).

Proof. Assume that (I) and (II) are fulfilled. It has been pointed out in Sec. 2.3 that the states $|\Psi_{\text{in}}\rangle$ maximizing the variance $\langle(\Delta H)^2\rangle_{\Psi_{\text{in}}}$ are the superpositions

$$|\Psi_{\text{in}}\rangle = \frac{1}{\sqrt{2}}(|\epsilon_{\text{max}}\rangle + e^{i\varphi}|\epsilon_{\text{min}}\rangle) \quad (88)$$

with $|\epsilon_{\text{max}}\rangle$ and $|\epsilon_{\text{min}}\rangle$ two eigenstates of H associated to ϵ_{max} and ϵ_{min} and $\varphi \in \mathbb{R}$. For such input states one has

$$|\dot{\Psi}_{\text{in}}\rangle = -i\Delta H|\Psi_{\text{in}}\rangle = -i\frac{\epsilon}{\sqrt{2}}(|\epsilon_{\text{max}}\rangle - e^{i\varphi}|\epsilon_{\text{min}}\rangle). \quad (89)$$

Furthermore,

$$\begin{aligned} |\Psi_x\rangle &= e^{-ix\Delta H}|\Psi_{\text{in}}\rangle \\ &= \frac{1}{\sqrt{2}}(e^{-ix\epsilon}|\epsilon_{\text{max}}\rangle + e^{i(x\epsilon+\varphi)}|\epsilon_{\text{min}}\rangle) \\ &= \cos(x\epsilon)|\Psi_{\text{in}}\rangle + \frac{1}{\epsilon}\sin(x\epsilon)|\dot{\Psi}_{\text{in}}\rangle. \end{aligned} \quad (90)$$

Since $\langle\Psi_{\text{in}}|\dot{\Psi}_{\text{in}}\rangle = 0$ and $\|\dot{\Psi}_{\text{in}}\|^2 = \langle(\Delta H)^2\rangle_{\Psi_{\text{in}}} = \epsilon^2$, the last expression in (90) is nothing but the arc of great circle (45) at time $\tau = x\epsilon$, i.e., $|\Psi_x\rangle = |\Psi_g(x\epsilon)\rangle$ with $|\Psi_g(\tau)\rangle$ a geodesic on the unit sphere $\mathcal{S}_{\mathcal{K}}$ (see Sec. 4.1). By condition (I) this geodesic is a horizontal geodesic, $|\Psi_g(\tau)\rangle = |\Psi_{g,V}(\tau)\rangle$. In view also of (69), one deduces that (a) is true. Now, plugging (88) and (89) into the expression of the geodesic Hamiltonian yields

$$H_{g,V} = |\epsilon_{\text{max}}\rangle\langle\epsilon_{\text{max}}| - |\epsilon_{\text{min}}\rangle\langle\epsilon_{\text{min}}| = \epsilon^{-1}\Pi(\Delta H)\Pi. \quad (91)$$

This shows that (I) & (II) $\Rightarrow$ (a) $\Rightarrow$ (b).

Reciprocally, assume that $|\dot{\Psi}_{\text{in}}\rangle \in \mathfrak{h}_{|\Psi_{\text{in}}\rangle}$ and that (b) is true. Since ϵ_{max} and ϵ_{min} are not degenerated,

$$\begin{aligned} \Pi(\Delta H)\Pi &= (\epsilon_{\text{max}} - \langle H \rangle_{\Psi_{\text{in}}})|\epsilon_{\text{max}}\rangle\langle\epsilon_{\text{max}}| \\ &\quad - (\langle H \rangle_{\Psi_{\text{in}}} - \epsilon_{\text{min}})|\epsilon_{\text{min}}\rangle\langle\epsilon_{\text{min}}|. \end{aligned} \quad (92)$$

Furthermore,

$$\begin{aligned} \epsilon H_{g,V} &= -i\epsilon\left(|\Psi_{\text{in}}\rangle\frac{\langle\dot{\Psi}_{\text{in}}|}{\|\dot{\Psi}_{\text{in}}\|} - \frac{|\dot{\Psi}_{\text{in}}\rangle}{\|\dot{\Psi}_{\text{in}}\|}\langle\Psi_{\text{in}}|\right) \\ &= \epsilon(|\epsilon_{+}\rangle\langle\epsilon_{+}| - |\epsilon_{-}\rangle\langle\epsilon_{-}|), \end{aligned} \quad (93)$$

where we have set

$$|\epsilon_{\pm}\rangle = \frac{1}{\sqrt{2}}\left(|\Psi_{\text{in}}\rangle \pm i\frac{|\dot{\Psi}_{\text{in}}\rangle}{\|\dot{\Psi}_{\text{in}}\|}\right). \quad (94)$$

Since $\langle\Psi_{\text{in}}|\dot{\Psi}_{\text{in}}\rangle = 0$, the vectors $|\epsilon_{\pm}\rangle$ are normalized and orthogonal. Thus, by (92) and (93), the equality in (b) implies $|\epsilon_{+}\rangle = e^{-i\varphi_{+}}|\epsilon_{\text{max}}\rangle$ and $|\epsilon_{-}\rangle = e^{-i\varphi_{-}}|\epsilon_{\text{min}}\rangle$, where $\varphi_{\pm}$ are real phases. It follows that $|\Psi_{\text{in}}\rangle$ is given by (88) up to an irrelevant phase factor, with $\varphi = \varphi_{+} - \varphi_{-}$, and

$$\begin{aligned} |\Psi_x\rangle &= e^{-ix\Delta H}|\Psi_{\text{in}}\rangle = e^{-ix\Pi(\Delta H)\Pi}|\Psi_{\text{in}}\rangle \\ &= e^{-ix\epsilon H_{g,V}}|\Psi_{\text{in}}\rangle = |\Psi_{g,V}(x\epsilon)\rangle \end{aligned} \quad (95)$$

(the second and last equalities follow from (88) and (69), respectively). Our hypothesis $|\dot{\Psi}_{\text{in}}\rangle \in \mathfrak{h}_{|\Psi_{\text{in}}\rangle}$ implies that $H_{g,V}$ is a geodesic Hamiltonian, i.e., $|\Psi_{g,V}(\tau)\rangle$ is a horizontal geodesic (see Property (i) of Sec. 3.3). Hence condition (I) is fulfilled. Furthermore, by (88) again, $\|\dot{\Psi}_{\text{in}}\|^2 = \langle(\Delta H)^2\rangle_{\Psi_{\text{in}}} = \epsilon^2$ is the maximal squared fluctuation of H . Thus condition (II) also holds. We have shown that (b) $\Rightarrow$ (a) $\Rightarrow$ (I) & (II). Finally, by projecting the equality (a) onto $\mathcal{E}_{\mathcal{H}}$, one obtains (87). $\square$

It is worth noting that the probe-ancilla input state $|\Psi_{\text{in}}\rangle$ is not necessarily entangled. To see this, let us vary the phase φ in (88) and observe that $|\Psi_{\text{in}}\rangle$ then moves on the horizontal geodesic as $|\Psi_{\text{in}}^0\rangle \rightarrow |\Psi_{\text{in}}^\varphi\rangle = e^{-i\varphi H_{g,V}/2}|\Psi_{\text{in}}^0\rangle$ up to an irrelevant phase factor, where $|\Psi_{\text{in}}^0\rangle$ is the input state corresponding to $\varphi = 0$. Recall from Sec. 4.3 that all geodesics $\gamma_{g,V}$ intersect the boundary $\partial\mathcal{E}_{\mathcal{H}}$ of quantum states. Therefore, if for instance the probe is a qubit, φ can be chosen such that $\rho_{\text{in}} = |\psi_{\text{in}}\rangle\langle\psi_{\text{in}}|$ is a pure state, that is, $|\Psi_{\text{in}}\rangle = |\psi_{\text{in}}\rangle|\alpha_{\text{in}}\rangle$ is a product state. In other words, albeit the superposition (88) is in general entangled, an appropriate phase choice makes it separable. Since preparing a probe and ancilla in an entangled state is challenging experimentally, this is a relevant observation. Let us stress that the aforementioned separability refers to a disentanglement between the probe and ancilla; if the probe consists of N qubits and H acts independently on each qubit, we shall see in Sec. 6.5 below that $|\Psi_{\text{in}}\rangle$ has maximal entanglement between the probe qubits. A phase choice such that the input state $|\Psi_{\text{in}}\rangle$ is a product state is also possible for higher-dimensional probes, but only for those geodesics such that the observable $M_{\rho\sigma,V}$ in (51) has two eigenvalues of multiplicities $n-1$ and 1. In fact, as argued in Sec. 4.3, this condition ensures that one of the intersection of $\gamma_{g,V}$ with $\partial\mathcal{E}_{\mathcal{H}}$ is a pure state.

The next theorem characterizes all system-ancilla Hamiltonians H generating horizontal geodesics, that is, coinciding (up to a numerical factor) with a geodesic Hamiltonian $H_{g,V}$ in a two-dimensional subspace. It shows that such Hamiltonians have two eigenvectors related to each other by a local unitary acting on the system.

Theorem 4. *Let $|\epsilon_1\rangle$ and $|\epsilon_2\rangle$ be two eigenstates of H with distinct eigenvalues ϵ_1 and ϵ_2 . If*

$$|\Psi_{\text{in}}\rangle = \frac{1}{\sqrt{2}}(|\epsilon_1\rangle + e^{i\varphi}|\epsilon_2\rangle) \quad (96)$$

then the unitary transformation $|\Psi_x\rangle = e^{-ix\Delta H}|\Psi_{\text{in}}\rangle$ is a horizontal geodesic if and only if $|\epsilon_2\rangle = U \otimes \mathbb{1}_A |\epsilon_1\rangle$ with U a local unitary acting on the system. In such a case $|\Psi_x\rangle = |\Psi_{g,V}(x\epsilon)\rangle$ with $\epsilon = (\epsilon_1 - \epsilon_2)/2$. In particular, conditions (I) and (II) hold if and only if $|\Psi_{\text{in}}\rangle$ is given by (88) and $|\epsilon_{\text{min}}\rangle = U \otimes \mathbb{1} |\epsilon_{\text{max}}\rangle$.

Proof. One deduces from $|\Psi_x\rangle = e^{-ix\Delta H}|\Psi_{\text{in}}\rangle$ and (96) that $|\Psi_{\text{in}}\rangle$ is given by (89) upon substituting $|\epsilon_{\text{max}}\rangle$ and $|\epsilon_{\text{min}}\rangle$ by $|\epsilon_1\rangle$ and $|\epsilon_2\rangle$. The horizontality condition $|\Psi_{\text{in}}\rangle = L_S \otimes \mathbb{1}_A |\Psi_{\text{in}}\rangle$ for some self-adjoint operator L_S such that $(L_S \otimes \mathbb{1}_A)\Psi_{\text{in}} = 0$ can be rewritten as

$$|\epsilon_2\rangle = e^{-i\varphi} \frac{\epsilon - iL_S}{\epsilon + iL_S} \otimes \mathbb{1}_A |\epsilon_1\rangle = U \otimes \mathbb{1}_A |\epsilon_1\rangle, \quad (97)$$

where U is a unitary operator acting on the probe and $\epsilon = (\epsilon_1 - \epsilon_2)/2$. Reciprocally, if $|\epsilon_2\rangle = U \otimes \mathbb{1}_A |\epsilon_1\rangle$ then

$$|\dot{\Psi}_{\text{in}}\rangle = -i\epsilon(1 - e^{i\varphi}U)(1 + e^{i\varphi}U)^{-1} \otimes \mathbb{1}_A |\Psi_{\text{in}}\rangle, \quad (98)$$

where it is assumed that $-e^{i\varphi}$ is not an eigenvalue of U (in such a way that $1 + e^{i\varphi}U$ is invertible). It is easy to show that the local operator in the right-hand side of (98) is self-adjoint. Hence $|\dot{\Psi}_{\text{in}}\rangle \in \mathfrak{h}_{|\Psi_{\text{in}}\rangle}$. $\square$

6.4 Optimal measurements

We now turn to the problem of determining the optimal measurement(s) on the probe maximizing the CFI. As explained in Sec. 6.1, these measurements are given in terms of the symmetric logarithmic derivative L_x of the output states $\rho_x = \gamma_{g,V}(x\epsilon)$. Let us fix a state σ on $\gamma_{g,V}$ such that ρ_x belongs to the geodesic arc between ρ_{in} and σ . Note that $\gamma_{g,V}$ is the same as the geodesic $\gamma_{g,V_x}^{\rho_x \rightarrow \sigma}$ starting at ρ_x and passing through σ translated in time by $-x\epsilon$ (see Appendix A for an explicit proof). Thus, by differentiating the latter geodesic at $\tau = 0$ one gets the tangent vector of $\gamma_{g,V}$ at $\tau_x = x\epsilon$. Making the substitutions $\rho \mapsto \rho_x$, $V \mapsto V_x$, and $\theta_V \mapsto \theta_V - \tau_x$ in (59), this gives

$$\dot{\gamma}_{g,V}(\tau_x) = \{\dot{X}_{\rho_x\sigma,V_x}, \rho_x\} \quad (99)$$

with

$$\dot{X}_{\rho_x\sigma,V_x} = \frac{1}{\sin(\theta_V - \tau_x)} (M_{\rho_x\sigma,V_x} - \cos(\theta_V - \tau_x)\mathbb{1}). \quad (100)$$

Plugging $\dot{\rho}_x = \epsilon \dot{\gamma}_{g,V}(\tau_x)$ into (74) and comparing with (99) yields

$$L_x = 2\epsilon \dot{X}_{\rho_x\sigma,V_x}. \quad (101)$$

In view of (100) and (101), the eigenprojectors of L_x are the eigenprojectors of $M_{\rho_x\sigma,V_x}$. The latter eigenprojectors, denoted hereafter by P_{i,V_x} , are related to the intersection states ρ_i of $\gamma_{g,V_x}^{\rho_x \rightarrow \sigma}$ with the boundary of quantum states (see Sec. 4.3 and Appendix B). More precisely, one has $\ker(\rho_i) = P_{i,V_x}\mathcal{H}$. But the ρ_i 's are independent of the state ρ_x on the geodesic $\gamma_{g,V}$ (in fact, $\gamma_{g,V_x}^{\rho_x \rightarrow \sigma}$ and $\gamma_{g,V}$ have the same intersections with $\partial\mathcal{E}_{\mathcal{H}}$). Therefore, the eigenprojectors P_{i,V_x} do not depend on the estimated parameter x . A more explicit proof that P_{i,V_x} only depend on the geodesic $\gamma_{g,V}$ is given in Appendix A. Recalling that the eigenprojectors of L_x form an optimal POVM, we conclude that

Theorem 5. *For output states given by (87), there exists a x -independent optimal POVM $\{M_i^{\text{opt}}\}$ given by the projective measurement with projectors $M_i^{\text{opt}} = P_{i,V}$ onto the kernels of the intersection states ρ_i of $\gamma_{g,V}$ with $\partial\mathcal{E}_{\mathcal{H}}$.*

More generally, thanks to the argument given in Sec. 6.1, a POVM $\{M_i^{\text{opt}}\}$ is optimal if and only if $\text{supp}(M_i^{\text{opt}}) \subset P_{i,V}\mathcal{H}$ up to permutations between the measurement operators.

As we have seen in Sec. 4.3, the number of eigenprojectors $P_{i,V}$ is equal to the number q_V of distinct eigenvalues of $M_{\rho\sigma,V}$. In particular, if $\gamma_{g,V}$ intersects $\partial\mathcal{E}_{\mathcal{H}}$ at a pure state, then the optimal measurement is a binary measurement consisting of $q_V = 2$ projectors, the first one being of rank $n - 1$ and the other of rank 1.

By Theorems 3 and 5, the CFI for the measurement outcome probabilities $p_{i|x}^{\text{opt}} = \text{tr } P_{i,V} \rho_x$ is equal to the QFI $4\langle(\Delta H)^2\rangle_{\Psi_{\text{in}}} = 4\epsilon^2$, being thus independent of the geodesic $\gamma_{g,V}$ in (87). One may ask oneself about the dependence on x and $\gamma_{g,V}$ of the distribution $\{p_{i|x}^{\text{opt}}\}_{i=1}^{q_V}$. Using (59) and the expression (B7) in Appendix B for the eigenvalues of $M_{\rho\sigma,V}$, one finds

$$p_{i|x}^{\text{opt}} = \frac{\sin^2(x\epsilon - \tau_i)}{\sin^2(\tau_i)} p_{i|0}^{\text{opt}}, \quad i = 1, \dots, q_V, \quad (102)$$

where $p_{i|0}^{\text{opt}} = \text{tr } P_{i,V} \rho$ and τ_i is the geodesic length between ρ and the i th intersection state ρ_i . For any geodesic $\gamma_{g,V}$ having a pure state intersection with the boundary ($q_V = 2$), choosing $\rho = \rho_1 = |\phi_1\rangle\langle\phi_1|$ so that $\tau_1 = 0$, $\tau_2 = \pi/2$, and $p_{2|0}^{\text{opt}} = 1$ (see Theorem 6), the binary optimal measurement yields a geodesic-independent distribution given by $\{p_{i|x}^{\text{opt}} = \sin^2(x\epsilon), p_{2|x}^{\text{opt}} = \cos^2(x\epsilon)\}$. Furthermore, for any value of q_V the conditional post-measurement states are independent of x , that is, $(p_{i|x}^{\text{opt}})^{-1} P_{i,V} \rho_x P_{i,V} = (p_{i|0}^{\text{opt}})^{-1} P_{i,V} \rho P_{i,V} \quad \forall x \in X$.

6.5 Heisenberg limit

We show in this subsection that the estimation error of the open probe undergoing a geodesic evolution can reach the Heisenberg scaling. To this end, we assume that a N -qubit probe is coupled to N ancilla qubits $A_1, \dots, A_N$. The total Hilbert space $\mathcal{K} = \mathbb{C}^{2^N} \otimes (\otimes_{\nu=1}^N \mathbb{C}_{A_\nu}^2)$ has dimension 2^{4N} . The ν th probe qubit S_ν is coupled to the ν th ancilla qubit A_ν by a Hamiltonian H_ν such that its eigenvectors $|e_{\nu,\pm}\rangle$ with maximal and minimal eigenvalues $e_{\nu,\pm}$ satisfy $|e_{\nu,-}\rangle = U_\nu \otimes \mathbb{1}_{A_\nu} |e_{\nu,+}\rangle$, where U_ν is a unitary acting on the ν th probe qubit. The total probe-ancilla Hamiltonian reads

$$H^{(N)} = \sum_{\nu=1}^N H_\nu, \quad (103)$$

where H_ν acts non-trivially on the ν th probe and ancilla qubits only. Then $H^{(N)}$ has two eigenvectors $|\epsilon_{\max}^N\rangle = \otimes_{\nu=1}^N |e_{\nu,+}\rangle$ and $|\epsilon_{\min}^N\rangle = \otimes_{\nu=1}^N |e_{\nu,-}\rangle$ associated to the highest and smallest eigenvalues

$$\epsilon_{\max}^N = \sum_{\nu=1}^N e_{\nu,+}, \quad \epsilon_{\min}^N = \sum_{\nu=1}^N e_{\nu,-}. \quad (104)$$

Let us consider the multipartite entangled input state

$$|\Psi_{\text{in}}^{(N)}\rangle = \frac{1}{\sqrt{2}} \left(\otimes_{\nu=1}^N |e_{\nu,+}\rangle + e^{i\varphi} \otimes_{\nu=1}^N |e_{\nu,-}\rangle \right), \quad (105)$$

where entanglement is between the N qubit pairs $(S_1 A_1), \dots, (S_N A_N)$. Since $|\epsilon_{\max}^N\rangle = U^{(N)} \otimes \mathbb{1}_A |\epsilon_{\min}^N\rangle$ with $U^{(N)} = \otimes_{\nu=1}^N U_\nu$, by Theorem 4 the unitary transformation

$$|\Psi_x^{(N)}\rangle = e^{-ixH^{(N)}} |\Psi_{\text{in}}^{(N)}\rangle = \otimes_{\nu=1}^N e^{-ixH_\nu} |\Psi_{\text{in}}^{(N)}\rangle \quad (106)$$

defines a horizontal geodesic on $\mathcal{S}_{\mathcal{K}}$. Thus the probe state $\rho_x^{(N)} = \text{tr}_A |\Psi_x^{(N)}\rangle \langle \Psi_x^{(N)}|$ follows a geodesic on $\mathcal{E}_{\mathbb{C}^{2^N}}$,

$$\rho_x^{(N)} = \gamma_{g,V}^{(N)}(x\epsilon_N) \quad , \quad \epsilon_N = \frac{\epsilon_{\max}^N - \epsilon_{\min}^N}{2}. \quad (107)$$

According to (85), the QFI of the probe is given by

$$\mathcal{F}_Q(\{\rho_x^{(N)}\}_{x \in X}) = 4\epsilon_N^2 = \left(\sum_{\nu=1}^N (e_{\nu,+} - e_{\nu,-}) \right)^2. \quad (108)$$

If the eigenenergies $e_{\nu,\pm}$ of the Hamiltonians H_ν are independent of ν , the QFI scales like N^2 , implying a minimal error $(\Delta x)_{\text{QCRB}} \sim N_{\text{meas}}^{-1/2} N^{-1}$ having the Heisenberg scaling. Let us point out that if the energy gap $2\epsilon = e_{\nu,+} - e_{\nu,-}$ of the ν th qubit-ancilla pair is twice the single qubit energy, then the QFI (108) is the same as the QFI obtained by using the ancilla qubits as additional probes, the state transformation being generated by $2N$ Hamiltonians acting on single qubits

and the input state being the maximally entangled $2N$ -qubit state. Our setup has the advantage that, for the same precision, one has to measure only half of the $2N$ qubits. An example of quantum circuit implementing this setup is shown in Fig. 3.

By Theorem 5, an optimal measurement is a joint projective measurement on the N probe qubits with projectors onto the kernels of the intersection states $\rho_i^{(N)}$ of the geodesic $\gamma_{g,V}^{(N)}$ with the boundary of the N -qubit state manifold.

7 Conclusions and perspectives

In this work we have studied the geodesics on the manifold of quantum states for the Bures distance. We have determined these geodesics and have shown that they are physical, as they correspond to quantum evolutions of an open system coupled to an ancilla. The corresponding system-ancilla coupling Hamiltonian has been derived explicitly. Examples of quantum circuits implementing some geodesics have been given. Furthermore, we have proven that the geodesics are optimal for single-parameter estimation in open quantum systems, where the unknown parameter is a phase shift multiplying a parameter-independent system-environment Hamiltonian. Actually, among all such Hamiltonians H with a fixed energy gap $2\epsilon = \epsilon_{\max} - \epsilon_{\min}$ between the maximal and minimal eigenvalues and all input state $|\Psi_{\text{in}}\rangle$ maximizing the QFI, i.e., such that $4\langle(\Delta H)^2\rangle_{\Psi_{\text{in}}} = 4\epsilon^2$, if one cannot measure the ancilla then the best precision for all parameter values is obtained when H and $|\Psi_{\text{in}}\rangle$ generate a geodesic evolution of the probe.

These results open the route to experimental observations of geodesics in multi-qubit quantum information platforms offering a high degree of control on the Hamiltonian. Such experimental realizations would be of interest for high-precision estimations in situations where only a part of these qubits can be measured.

The methods developed in this paper, which are borrowed from Riemannian geometry, are expected to be applicable as well to non ideal quantum metrology setups. For instance, when the coupling with the environment provokes energy losses and dephasing, additional couplings with engineered reservoirs could be tailored to modify the state transformation so that it becomes closer to a geodesic. This would increase the precision of the estimation by reducing the amount of information on the parameter lost in the environment. Alternatively, one could investigate whether H can be steered to a geodesic Hamiltonian by using external controls acting either on the probe or on its environment.

Another potential field of application of the Bures geodesics is incoherent quantum control. In order to efficiently steer a quantum mixed state ρ to a given desired state σ , an idea is to adjust the control param-

eters in such a way as to follow as closely as possible the shortest geodesic joining ρ and σ [47]. Among other directions worth exploring is the relation between the geodesic evolutions and the quantum speed limit in open systems [48].

The present work can be contextualized as belonging to an emerging broader research topic. Information geometry has been developed in the last decades by Amari and coworkers [49, 50] in an attempt to use concepts and methods from Riemannian geometry in information theory. It has been successfully applied to many fields, such as machine learning, signal processing, optimization, statistics, and neurosciences. The application of this approach to quantum information processing remains largely unexplored. It will hopefully open new challenging perspectives.

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A Properties of the operator $M_{\rho\sigma,V}$

The operator $M_{\rho\sigma,V} = \rho^{-1/2}|\sqrt{\sigma}\sqrt{\rho}|\rho^{-1/2}$ in the expression (59) of the Bures geodesics has the following properties:

- (a) $M_{\rho\sigma,V} \rho M_{\rho\sigma,V} = \sigma$;
- (b) $\text{tr} \rho M_{\rho\sigma,V} = \cos \theta_V$, $\text{tr} \rho M_{\rho\sigma,V}^2 = 1$;
- (c) $M_{\sigma\rho,\tilde{V}} = M_{\rho\sigma,V}^{-1}$ and $M_{\rho\sigma,V} \rho = \sigma M_{\sigma\rho,\tilde{V}}$, where $\tilde{V} = U_{\sigma\rho} V U_{\sigma\rho}^\dagger$.

Properties (a) and (b) follow from the definition of $M_{\rho\sigma,V}$ and from (58). The first identity in (c) follows from the equality $M_{\rho\sigma,V} = \sqrt{\sigma} U_{\sigma\rho} V \rho^{-1/2}$, see (51), and the fact that the unitary $U_{\sigma\rho}$ in the polar decomposition of $\sqrt{\rho}\sqrt{\sigma}$ is equal to the adjoint of $U_{\sigma\rho}$ (recall that if $O = U|O|$ then $O^\dagger = U^\dagger|O|$). The second identity is then deduced from (a). Observe that (a) is equivalent to $\gamma_{g,V}(\theta_V) = \sigma$, see (59). Property (b) can be used to show that $\text{tr} \gamma_{g,V}(\tau) = 1$ for all τ (as it should be since $\gamma_{g,V}(\tau)$ is a quantum state). Property (c) insures that the geodesic joining σ to ρ , obtained by exchanging ρ and σ in (59), coincides with the time-reversed geodesic $\gamma_{g,\tilde{V}}(\theta_V - \tau)$. By using the self-adjointness and unitarity of V and $[\Lambda_{\sigma\rho}, V] = 0$, it is easy to show that $\tilde{V}$ enjoys the same properties, the commutation being with $\Lambda_{\sigma\rho} = |\sqrt{\rho}\sqrt{\sigma}| = U_{\sigma\rho} \Lambda_{\sigma\rho} U_{\sigma\rho}^\dagger$.

The next property tells us how $M_{\rho\sigma,V}$ is transformed as one moves ρ along the geodesic $\gamma_{g,V}$, keeping σ fixed. For any invertible state $\rho_t = \gamma_{g,V}(t)$ on $\gamma_{g,V}$, with $0 \leq t \leq \theta_V$, one has

$$(d) \quad M_{\rho\sigma,V} = M_{\rho_t\sigma,V_t} X_{\rho\sigma,V}(t),$$

where $X_{\rho\sigma,V}(t)$ is given by (60) and V_t is some self-adjoint unitary operator commuting with $\Lambda_{\sigma\rho_t} = |\sqrt{\sigma}\sqrt{\rho_t}|$. This formula is related to the fact that the geodesics joining ρ_t and σ are the geodesics joining ρ and σ shifted in time,

$$\gamma_{g,V_t}^{(t)}(\tau) = \gamma_{g,V}(t + \tau), \quad 0 \leq \tau \leq \theta_V - t. \quad (\text{A1})$$

We will prove in Appendix B that the spectrum of V_t is constant in time save at the intersection times of $\gamma_{g,V}$ with the boundary $\partial\mathcal{E}_{\mathcal{H}}$, where some eigenvalues of V_t may jump from -1 to $+1$. In particular, if $V = \mathbb{1}$ then $V_t = \mathbb{1}$ for $0 \leq t \leq \theta_1$.

Formula (d) can be proven directly from (51) and (59), but it is simpler to derive it from the properties of horizontal geodesics on the hypersphere $\mathcal{S}_{\mathcal{K}}^{\text{inv}}$. In fact, it is clear geometrically that the arc of great circle joining $|\Psi_t\rangle = |\Psi_g(t)\rangle$ to $|\Phi_V\rangle$ has length $\theta_V - t$ and is contained in the arc of great circle joining $|\Psi\rangle$ to $|\Phi_V\rangle$, so that it is parametrized by

$$|\Psi_g^{(t)}(\tau)\rangle = |\Psi_g(t + \tau)\rangle, \quad 0 \leq \tau \leq \theta_V - t. \quad (\text{A2})$$

Since $|\Psi_g(\tau)\rangle$ is a horizontal geodesic, its tangent vector $|\dot{\Psi}_t\rangle$ at $|\Psi_t\rangle$ is horizontal (property (i) of Sec. 3.3).

According to the result of Sec. 4.1, this is equivalent to

$$|\Phi_V\rangle = M_{\rho_t\sigma,V_t} \otimes \mathbb{1}_A |\Psi_t\rangle \quad (\text{A3})$$

for some self-adjoint unitary V_t commuting with $\Lambda_{\sigma\rho_t}$. By (50), (55), and (60), one has

$$|\Psi_t\rangle = |\Psi_g(t)\rangle = X_{\rho\sigma,V}(t) \otimes \mathbb{1}_A |\Psi\rangle. \quad (\text{A4})$$

Plugging (A4) into (A3) one gets

$$|\Phi_V\rangle = M_{\rho_t\sigma,V_t} X_{\rho\sigma,V}(t) \otimes \mathbb{1}_A |\Psi\rangle = M_{\rho\sigma,V} \otimes \mathbb{1}_A |\Psi\rangle. \quad (\text{A5})$$

One easily shows that the second equality is equivalent to (d) (for instance, one may rely on (47)). Furthermore, (A2) implies (A1) since the projection on $\mathcal{E}_{\mathcal{H}}^{\text{inv}}$ of the horizontal geodesic $|\Psi_g^{(t)}(\tau)\rangle$ is the Bures geodesic joining ρ_t and σ with unitary V_t .

An important consequence of (d) for applications to quantum metrology is the following. As shown in Appendix B, $X_{\rho\sigma,V}(t)$ is invertible when ρ_t is invertible, i.e., when t is not an intersection time of $\gamma_{g,V}$ with $\partial\mathcal{E}_{\mathcal{H}}$. In such a case $M_{\rho_t\sigma,V_t} = M_{\rho\sigma,V} X_{\rho\sigma,V}(t)^{-1}$ is a function of the self-adjoint operator $M_{\rho\sigma,V}$ (recall that $X_{\rho\sigma,V}(t)$ is a function of $M_{\rho\sigma,V}$, see (60)). Thus the eigenprojectors of $M_{\rho_t\sigma,V_t}$ are t -independent and coincide with the eigenprojectors of $M_{\rho\sigma,V}$.

B Intersections of the geodesics with the boundary of quantum states

In this appendix we study the intersections of the Bures geodesics with the boundary of quantum states $\partial\mathcal{E}_{\mathcal{H}}$. As explained in the main text, we consider the extensions of the geodesic arcs $\gamma_{g,V}$ joining two states ρ and $\sigma \in \mathcal{E}_{\mathcal{H}}^{\text{inv}}$ to the time interval $[0, \pi]$, given by (59) with $0 \leq \tau \leq \pi$. These extensions are closed geodesic curves, which are denoted by the same symbol $\gamma_{g,V}$. Recall that these curves depend on a self-adjoint unitary operator V commuting with $\Lambda_{\sigma\rho}^2 = \sqrt{\rho}\sigma\sqrt{\rho}$. The arc length of $\gamma_{g,V}$ between ρ and σ is denoted by θ_V (see Theorem 1).

Theorem 6. *One has*

- (i) $\gamma_{g,V}$ intersects q_V times $\partial\mathcal{E}_{\mathcal{H}}$, where q_V is the number of distinct eigenvalues of the operator $M_{\rho\sigma,V}$ in (51). While the shortest geodesic γ_g does not intersect $\partial\mathcal{E}_{\mathcal{H}}$ between ρ and σ , i.e., $\gamma_g([0, \theta_1]) \subset \mathcal{E}_{\mathcal{H}}^{\text{inv}}$, the other geodesics with $V \neq \mathbb{1}$ do so at least once. More precisely, the number of intersections of $\gamma_{g,V}([0, \theta_V])$ with $\partial\mathcal{E}_{\mathcal{H}}$ is equal to the multiplicity of the eigenvalue -1 of V .
- (ii) The intersection points ρ_i of $\gamma_{g,V}$ with $\partial\mathcal{E}_{\mathcal{H}}$ have ranks $n - m_{i,V}$ and supports $(\mathbb{1} - P_{i,V})\mathcal{H}$, where $m_{i,V}$ and $P_{i,V}$ are the multiplicities of the eigenvalues and the spectral projectors of $M_{\rho\sigma,V}$, re-

spectively. In particular,

$$\sum_{i=1}^{q_V} \dim(\ker \rho_i) = n. \quad (\text{B6})$$

(iii) Given an invertible state $\rho \in \mathcal{E}_{\mathcal{H}}^{\text{inv}}$ and a pure state $|\phi_1\rangle$ such that $\langle \phi_1 | \rho | \phi_1 \rangle > 0$, there are exactly two geodesics passing through ρ and intersecting $\partial\mathcal{E}_{\mathcal{H}}$ at $\rho_1 = |\phi_1\rangle\langle\phi_1|$, namely the shortest geodesic $\gamma_{g,\rho \rightarrow \rho_1}(\tau)$ joining ρ and ρ_1 and its time reversal $\gamma_{g,\rho \rightarrow \rho_1}(\pi - \tau)$. Moreover, $\gamma_{g,\rho \rightarrow \rho_1}$ intersects twice $\partial\mathcal{E}_{\mathcal{H}}$; the other intersection point ρ_2 has rank $n-1$ and support orthogonal to $|\phi_1\rangle$, being therefore separated from ρ_1 by a geodesic distance $\pi/2$.

The results (i) and (ii) have been proven in Ref. [34] in the particular case $V = \mathbb{1}$. It follows from (ii) that $\gamma_{g,V}$ intersects $\partial\mathcal{E}_{\mathcal{H}}$ at a pure state if and only if $M_{\rho\sigma,V}$ has two eigenvalues of multiplicities $n-1$ and 1. Note that this is always the case for $n=2$ (for a qubit, $\partial\mathcal{E}_{\mathcal{H}}$ is the set of pure states).

For a qutrit ($n=3$), there are up to time-reversal four geodesics passing through two generic states $\rho > 0$ and $\sigma > 0$, where by generic we mean that $\Lambda_{\sigma\rho} = |\sqrt{\sigma}\sqrt{\rho}|$ has a non-degenerate spectrum, see the discussion after Theorem 1. The shortest geodesic γ_g joining ρ and σ , obtained for $V = \mathbb{1}$, does not intersect $\partial\mathcal{E}_{\mathcal{H}}$ between these two states. Its time-reversal is the geodesic obtained for $V = -\mathbb{1}$. The three other geodesics correspond to V having spectrum $\{1, 1, -1\}$ (or $\{-1, -1, 1\}$ for their time-reversal). They intersect the boundary once (twice for the time-reversal) between ρ and σ . If $M_{\rho\sigma,V}$ has non-degenerated eigenvalues then $\gamma_{g,V}$ has $q_V = 3$ intersections ρ_i with $\partial\mathcal{E}_{\mathcal{H}}$, which have rank 2.

Proof. (i) To simplify the notation we do not write explicitly the dependence on ρ , σ , and V of the operators $M_{\rho\sigma,V}$, $X_{\rho\sigma,V}$, etc. Following the arguments of [34], we observe that in view of (59), $\gamma_{g,V}(\tau) \in \partial\mathcal{E}_{\mathcal{H}}$ if and only if $\det \gamma_{g,V}(\tau) = \det X(\tau)^2 \det \rho = 0$, that is, $\det X(\tau) = 0$. The last determinant is the characteristic polynomial of M , see (60). Thus $\gamma_{g,V}$ intersects q times $\partial\mathcal{E}_{\mathcal{H}}$, at times $\tau_1 < \dots < \tau_q$ given by

$$\frac{\sin(\theta_V - \tau_i)}{\sin \tau_i} = -\mu_i \Leftrightarrow \cotan \tau_i = \frac{\cos \theta_V - \mu_i}{\sin \theta_V}, \quad (\text{B7})$$

where $\mu_1 < \dots < \mu_q$ are the distinct eigenvalues of M . If $V = \mathbb{1}$ then $M > 0$ and thus $\mu_1 > 0$. Hence $\cotan \tau_1 < \cotan \theta_1$, so that the first intersection time satisfies $\tau_1 > \theta_1$. This tells us that the shortest geodesic arc $\gamma_g([0, \theta_1])$ starting at ρ and ending at σ is contained in $\mathcal{E}_{\mathcal{H}}^{\text{inv}}$, i.e., it does not intersect $\partial\mathcal{E}_{\mathcal{H}}$. In contrast, let us show that if $V \neq \mathbb{1}$ then M has at least one negative eigenvalue $\mu_1 < 0$. In fact, V has at least one eigenvalue $v_k = -1$. Denote by

$|\varphi_k\rangle$ a common eigenvector of V and $\Lambda = |\sqrt{\sigma}\sqrt{\rho}|$ for the eigenvalues v_k and λ_k , respectively. Then

$$\langle \varphi_k | \sqrt{\rho} M \sqrt{\rho} | \varphi_k \rangle = \langle \varphi_k | \Lambda V | \varphi_k \rangle = -\lambda_k < 0. \quad (\text{B8})$$

By the variational principle it follows that $\mu_1 < 0$. Hence M has $s \geq 1$ negative eigenvalues $\mu_1 < \dots < \mu_s < 0$. One deduces from (B7) that $\cotan \tau_i > \cotan \theta_V$ and thus $\tau_i < \theta_V$ for $i = 1, \dots, s$. A reversed inequality holds for $i > s$. This shows that $\gamma_{g,V}$ intersects the boundary s times on its part between ρ and σ . The fact that s is equal to the multiplicity of the eigenvalue -1 of V follows from a similar argument, using the min-max theorem for self-adjoint operators.

(ii) Let us now prove that the intersection states $\rho_i = \gamma_g(\tau_i) \in \partial\mathcal{E}_{\mathcal{H}}$ have ranks $r_i = n - m_i$ and supports

$$\text{supp}(\rho_i) = Q_i \mathcal{H} = [\ker(M - \mu_i)]^\perp, \quad (\text{B9})$$

where m_i and P_i are the multiplicity and spectral projector of M for the eigenvalue μ_i and $Q_i = \mathbb{1} - P_i$. We first note that

$$X_i = X(\tau_i) = \frac{\sin \tau_i}{\sin \theta} (M - \mu_i) \quad (\text{B10})$$

has rank r_i and support $Q_i \mathcal{H}$, so that $X_i = Q_i X_i Q_i$. But

$$\rho_i = X_i \rho X_i, \quad (\text{B11})$$

hence $\ker(\rho_i) \supset \ker(X_i)$. Reciprocally, let $|\varphi\rangle \in \ker(\rho_i)$. Then $\rho X_i |\varphi\rangle \in P_i \mathcal{H}$, that is, $Q_i \rho Q_i X_i |\varphi\rangle = 0$. Since $Q_i \rho Q_i$ is invertible on $Q_i \mathcal{H}$ (recall that $\rho > 0$), one has $|\varphi\rangle \in \ker(X_i)$. This implies that $\ker(\rho_i) = \ker(X_i) = P_i \mathcal{H}$ and thus $\text{supp}(\rho_i) = Q_i \mathcal{H}$, as announced above.

(iii) Let $\gamma_{g,V}$ be a geodesic starting at ρ and intersecting the boundary at $\rho_1 = |\phi_1\rangle\langle\phi_1|$. Thanks to (B9) one has

$$M - \mu_1 = \langle M - \mu_1 \rangle_{\phi_1} |\phi_1\rangle\langle\phi_1|. \quad (\text{B12})$$

Using (B7) and (B12) one obtains

$$\begin{aligned} \langle M - \mu_1 \rangle_{\phi_1} \langle \rho \rangle_{\phi_1} &= \text{tr}(M - \mu_1) \rho \\ &= \text{tr} M \rho - \cos \theta + \sin \theta \cotan \tau_1 \\ &= \sin \theta \cotan \tau_1, \end{aligned} \quad (\text{B13})$$

where the last equality follows from property (b) of Appendix A. Furthermore, equating $X_1 \rho X_1$ with $\rho_1 = |\phi_1\rangle\langle\phi_1|$ and using (B10) and (B12), one gets $\cos \tau_1 = \pm \langle \rho \rangle_{\phi_1}^{1/2}$. For any choice of the operator V , τ_1 is thus either equal to $d_B(\rho, \rho_1) = \arccos(\langle \rho \rangle_{\phi_1}^{1/2})$ or to π minus this distance. We can now express μ_1 and $\langle M - \mu_1 \rangle_{\phi_1}$ in terms of θ and τ_1 , replace these expressions into (B12), and use (60) in the main text to obtain

$$X(\tau) = \frac{1}{\sin \tau_1} \left(\sin(\tau_1 - \tau) \mathbb{1} + \frac{\sin \tau}{\cos \tau_1} |\phi_1\rangle\langle\phi_1| \right). \quad (\text{B14})$$

Observe that $X(\tau)$ depends on $|\phi_1\rangle$ and τ_1 but not on θ . Therefore, there are exactly two geodesic arcs $\gamma_{g,V}(\tau) = X(\tau)\rho X(\tau)$ starting at ρ and intersecting $\partial\mathcal{E}_{\mathcal{H}}$ at ρ_1 . The first one has length $\tau_1 = d_B(\rho, \rho_1)$ (shortest geodesic $\rho \rightarrow \rho_1$), the second one has length $\tau_1 = \pi - d_B(\rho, \rho_1)$ (time-reversed geodesic). The other affirmations in (iii) are direct consequences of (ii). Note that if $\langle \rho \rangle_{\phi_1} = 0$ then there are no geodesic joining ρ to ρ_i because in such a case (B10) and (B12) imply that $X_1\rho X_1$ vanish, in contradiction with $X_1\rho X_1 = \rho_1$. $\square$

Let us now apply Theorem 6 and a continuity argument to determine the self-adjoint unitary operators V_t appearing in property (d) and Eq. (A1) of Appendix A. Recall that V_t is associated to the time-shifted geodesic $\gamma_{g,V_t}^{(t)}(\tau) = \gamma_{g,V}(t+\tau)$ joining ρ_t and σ and that V_t commutes with $\Lambda_{\sigma\rho_t} = |\sqrt{\sigma}\sqrt{\rho_t}|$. Denoting as above by $\tau_1 < \tau_2 < \dots < \tau_q$ the intersection times of $\gamma_{g,V}$ with $\partial\mathcal{E}_{\mathcal{H}}$, we first assume that $0 \leq t < \tau_1$. One deduces from property (d) that

$$V_t = \Lambda_{\sigma\rho_t}^{-1} \sqrt{\rho_t} M_{\rho\sigma,V} X_{\rho\sigma,V}(t)^{-1} \sqrt{\rho_t}. \quad (\text{B15})$$

Here, we have used that $\Lambda_{\sigma\rho_t}$ and $X_{\rho\sigma,V}(t)$ are invertible for $0 \leq t < \tau_1$ (in fact, for $t \neq \tau_i$ one has $\det \rho_t = (\det X_{\rho\sigma,V}(t))^2 \det \rho \neq 0$, see the proof of Theorem 6). Furthermore, $\Lambda_{\sigma\rho_t}^{-1}$ and $X_{\rho\sigma,V}(t)^{-1}$ are continuous in time in view of the continuity of ρ_t and of (60), respectively. It follows that V_t is continuous in time on $[0, \tau_1)$. Thus its eigenvalues $v_k(t) \in \{-1, 1\}$ are time-independent on this interval and $V_t = \sum_k v_k |\varphi_k(t)\rangle \langle \varphi_k(t)|$ for any $t \in [0, \tau_1)$, where v_k are the eigenvalues of $V = V_0$ and $\{|\varphi_k(t)\rangle\}_{k=1}^n$ is a time-continuous orthonormal basis diagonalizing $\Lambda_{\sigma\rho_t}$. In particular, if $V = \mathbb{1}$ then $V_t = \mathbb{1}$ for all $t \in [0, \theta_1]$ (in fact, in such a case $\tau_1 > \theta_1$ by Theorem 6(i)). Eq. (A1) then ensures that $\gamma_{g,V_t}^{(t)}(\tau) = \gamma_g(t+\tau)$ is the shortest geodesic arc joining ρ_t and σ and has length $d_B(\rho_t, \sigma) = \theta_1 - t$ with $t = d_B(\rho, \rho_t)$. This is consistent with the additivity property of the distance,

$$d_B(\rho, \sigma) = d_B(\rho, \rho_t) + d_B(\rho_t, \sigma), \quad \rho_t \in \gamma_g([0, \theta_1]). \quad (\text{B16})$$

On the other hand, if $\tau_i < t < \tau_{i+1} < \theta_V$ then the number of intersections with $\partial\mathcal{E}_{\mathcal{H}}$ of the time-shifted geodesic arc $\gamma_{g,V_t}^{(t)}([0, \theta_V - t])$ is reduced by i as compared to the number of intersections of $\gamma_{g,V}([0, \theta_V])$ with $\partial\mathcal{E}_{\mathcal{H}}$. According to Theorem 6(i), the multiplicity of the eigenvalue -1 of V_t equals $s-i$, where s is the multiplicity for V . By the same argument as above, the eigenvalues of V_t and their multiplicities are constant between τ_i and τ_{i+1} , but the multiplicities jump by one at the intersection times. In particular, the identity (B16) does not hold for $t > \tau_1$.